THE WATER QUALITY ANALYSIS SIMULATION PROGRAM, WASP5

PART B:

THE WASP5 INPUT DATASET

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by

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CHAPTER 1

INTRODUCTION

1.1 GENERAL CONSIDERATIONS

This section describes the input required to run the WASP5 water quality program. The user should be cautioned about potential changes to the dataset or manual that may accompany version updates of the software. The printed manual may become dated as enhancements are made or errors are identified and corrected. Please download the latest manual accompanying the current version of WASP5.

To arrange the input into a logical format, WASP5 data are divided into 10 groups, A through J:

A - Model Identification and Simulation Control

B - Exchange Coefficients

C - Volumes

D - Flows

E - Boundary Concentrations

F - Waste Loads

G - Environmental Parameters

H - Chemical Constants

I - Time Functions

J - Initial Conditions

The following is a brief explanation of each data group:

DATA GROUP A provides for descriptive model identification and contains simulation control options. The user must specify the number of segments and the number of systems. The user must also specify calculational time steps and print intervals here.

DATA GROUP B contains dispersive exchange information. Dispersion occurs between segments and along a characteristic length. Dispersion coefficients vary with time in a piecewise linear time function.

DATA GROUP C supplies initial segment volume information, and information on the segment type and underlying segment numbers. Hydraulic geometry information can be given to derive segment average depth and velocity as a function of flow. These

values are used in reaeration and volatilization calculations only (not in the basic transport calculations.)

WASP 5.2-MDEP (version 5.2-Maine DEP, November 2001) revised for Maine Department of Environmental Protection (MDEP) provides two options for computation of tidal flow and bottom area based on simple tidal prism flow or depth-time functions in estuarine environments specified by a new flag IDOPT in Record-1 of Data Group C.

DATA GROUP D supplies flow and sediment transport information between segments. Flows may be contained in the WASP input dataset, or may be imported from an external hydrodynamic file. Flows in the WASP5 input dataset vary with time following a piecewise linear time function.

DATA GROUP E supplies concentrations for each system at the boundaries. All system concentrations must be supplied for each boundary. Boundary concentrations vary with time in a piecewise linear time function.

DATA GROUP F defines the waste loads and segments that receive the waste loads for both point and diffuse sources. Point source loads vary with time in a piecewise linear time fuction. Nonpoint source loads vary with time in a daily step function.

WASP 5.2-MDEP includes an additional Data Block F3, which provides an alternative input option for input of steady NPS loads. Steady NPS loads are expressed in terms of mass load.

DATA GROUP G contains appropriate environmental characteristics of the water body. These parameters are spatially variable, varying with each model segment.

WASP 5.2-MDEP has fourteen additional parameters available for EUTRO5 simulations. WASP 5.2-MDEP allows algal growth rate, algal respiration rate, algal die-off rate, zooplankton grazing rate, nitrogenous BOD decay rate, and carbonaceous BOD decay rate constants to vary by reach. Card Group H is used to specify these constant(s) at once for all segments. Thus, the user has two options for specifying these inputs: for constants that are constant over the entire model domain, Card Group H would be used just as is done in WASP5. For constants that are varied by reach, Card Group G would be used instead. Specifying constants in both Card Groups G and H triggers an error message.

DATA GROUP H contains appropriate chemical characteristics or constants. Constants in WASP remain constant in both time and space. WASP 5.2-MDEP includes eighteen additional cnstants for macrophytes/periphyton simulation and five additional cnstants for calculaiion of light intensity.

DATA GROUP I contains appropriate environmental or kinetic time functions.

Time functions 24 to 35 (TEMP5 to TEMP16) are an additional twelve temperature functions available for parameter TMPFN and time function 36 (TFBOD) is added for parameter FBOD to allow benthic CBOD fluxes in WASP 5.2-MDEP.

DATA GROUP J contains initial concentrations for each segment and each system, along with dissolved fractions and the density of solids systems.

The input dataset is a formatted ASCII file. The user must carefully place input data in the appropriate fields, and be sure to right justify integers.

Dimensional Limits

The new dimensional limits set in WASP 5.2-MDEP are presented below.

Variables/Parameters	New Dimensional Limits	Variable in WASP.CMN
Number of point sources	50	WK
Number of reaches	300	SG
Number of nonpoint sources	200	WK
Number of flow time functions	18-per flow field	MNI
Number of dispersion time functions	10	MNI
Number of boundaries	10	BC

1.2 THE EUTROPHICATION MODEL

EUTRO5 requires the same input format as the basic WASP5 model. This format is explained in detail in the chapters below. This section summarizes the variables needed specifically for EUTRO5.

As described in detail in Chapter 5, the 10 systems for eutrophication modeling are ammonia nitrogen, nitrate nitrogen, inorganic phosphorus, phytoplankton carbon, carbonaceous BOD, dissolved oxygen, organic nitrogen, organic phosphorus,

periphyton, and salinity. In WASP5, salinity is specified as an Environmental Parameter in the EUTROWASP Data Group G input.

Periphyton is included as a ninth and salinity as a tenth system variable that are computed based on boundary conditions and computed transport in MDEP WASP. If the user specifies NOSYS = 8 on Record 4, which is the WASP5 specification for the eutrophication model, then neither periphyton nor salinity are included as system variables and the program default to WASP5 operation. If the user specifies 10, then the program ignores the SAL(ISEG) input in Data Group G. Table 1 summarizes these systems and their use in seven discrete levels of complexity.

The user should note that these discrete levels of complexity are suggestive only. The user may choose to simulate any combination of these variables using any combination of the parameter functions and values described below. In fact, during calibration, the user may choose to simulate only one variable, such as CBOD, while bypassing (and thus holding constant) all other variables.

The periphyton system should not be specified without also specifying the phytoplankton system. Sunlight is calculated for the phytoplankton system only, but used for the periphyton system. If the periphyton system is specified without the phytoplankton system, there are not valid sunlight inputs for the periphyton calculation.

Table 1 EUTRO5 Systems and Levels of Complexity

System Number	Symbol	Name	Use in Complexity Level 1	2	3	4	5	6	7
1	NH3	Ammonia nitrogen		X	X	X	X	X	X
2	NO3	Nitrate nitrogen			X	X	X	X	X
3	PO4	Inorganic phosphorus				X	X	X	X
4	CHL	Phytoplankton carbon				X	X	X	X
5	CBOD	Carbonaceous BOD	X	X	X	X	X	X	X
6	DO	Dissolved oxygen	X	X	X	X	X	X	X
7	ON	Organic nitrogen			X	X	X	X	X
8	OP	Organic phosphorus				X	X	X	X
9	MAC	Periphyton carbon							X
10	SAL	Salinity	*	*	*	*	*	*	*

Complexity Level	Explanation
1	"Streeter-Phelps" BOD-DO with SOD
2	"Modified Streeter-Phelps" with NBOD
3	Linear DO balance with nitrification
4	Simple eutrophication
5	Intermediate eutrophication
6	Intermediate eutrophication with benthos
7	Intermediate eutrophication with periphyton

* Salinity can be added independent of the complexity level

1.3 THE TOXIC CHEMICAL MODEL

TOXI5 requires the same input format as the basic WASP5 model. This format is explained in detail in the chapters below. This section summarizes the variables needed specifically for TOXI5.

As described in Chapter 7, the 6 systems for toxicant modeling are chemical 1, solids fraction 1, solids fraction 2, solids fraction 3, chemical 2, and chemical 3. Table 2 summarizes these systems and their use in several discrete levels of complexity. These levels of complexity describe possible approaches to simulating solids, equilibrium reactions, and kinetic reactions. They are suggestive only. The user may choose to simulate any combination of these variables using any combination of the parameter functions and values described below.

Table 2 TOXI5 Systems and Levels of Complexity

System Number	Symbol	Name	Levels of Complexity for: Solids 1, 2	Solids 3	Solids 4	Kinetics 1-3	Kinetics 4
1	C_1	Chemical 1	X	X	X	X	X
2	S_1	Solid 1		X	X		
3	S_2	Solid 2			X		
4	S_3	Solid 3			X		
5	C_2	Chemical 2					X
6	C_3	Chemical 3					X

Complexity Level	Explanation
Solids 1	Descriptive Solids concentration field
Solids 2	Descriptive solids concentration field with specific solids transport rates
Solids 3	Simulated total solids
Solids 4	Three simulated solids types
Equil 1	Constant partition coefficient
Equil 2	Spatially-variable partition coefficients
Equil 3	Hydrophobic sorption
Equil 4	Solids-dependent partitioning
Equil 5	Sorption plus ionic speciation
Kinetic 1	Constant half lives or rate constants
Kinetic 2	Spatially-variable rate constants
Kinetic 3	Second order rates
Kinetic 4	Transformation products

CHAPTER 2

DATA GROUP A: MODEL IDENTIFICATION AND SIMULATION CONTROL

Basic simulation information is provided in Data Group A, beginning with titles and descriptions in Records 1 and 2. The number of systems (state variables) and segments are specified in Record 4. Calculational time steps are provided in Records 6 and 7, and print intervals in Records 8 and 9. System bypass options are set in Record 10.

2.1 RECORD FORMATS

Record 1--Title of Simulation (A5, A75)

SIMTYP = type of simulation; TOXI5 = toxics dataset; EUTRO = eutrophication dataset. (A5)

TITLE1 = descriptive title of simulation. (A75)

Record 2--Description of Simulation (A80)

TITLE2 = description of simulation. (A80)

Record 3--Record 4 Names (A80)

HEADER = names of Record 4 variables, positioned properly; for user convenience only. (A80)

Record 4--Simulation Control Parameters (7I5, 2F5.0, F3.0, F2.0)

NOSEG = number of segments in model network. (I5)

NOSYS = number of model systems (state variables). (I5)

ICFL = flag controlling use of restart file; 0 = neither read from nor write to restart file (initial conditions located in input file); 1 = write final simulation results to restart file (initial conditions located in input file); 2 = read initial conditions from restart file created by earlier simulation, and write final simulation results to new restart file. (I5)

MFLAG = flag controlling messages printed on screen during simulation; 0 = all messages printed;

1 = simulation time only printed; 2 = all messages are suppressed. (I5)

JMASS = system number for which mass balance analysis will be performed; 0 = no mass balance table generated. (I5)

NEGSLN = negative solution option; 0 = prevents negative solutions; 1 = allows negative solutions. (I5)

INTYP = time step option; 0 = user inputs time step history; 1 = model calculates time step. (I5)

ADFAC = advection factor; 0 = backward difference; 0.5 = central difference; 0-0.4 recommended. (F5.0)

ZDAY = day at beginning of simulation; 1 is first day. (F5.0)

ZHR = hour at the beginning of simulation. (F3.0)

ZMIN = minute at the beginning of simulation. (F2.0)

TFLG = switch controlling generation of transport file; 0 = generate file; 1 = do not generate file. (I5)

Record 5--Runtime Print Segments (6I5)

ISEGOUT = up to six segment numbers to display at runtime; if there are six or more segments in the model network, the user should specify six print segment numbers. (I5)

Record 6--Number of Time Steps (I5)

NOBRK = number of different model time steps (I5)

Record 7--Time Steps (4(F10.0, F10.0))

DTS(I) = time step to be used until time T(I), days. (F10.0)

T(I) = time up to when time step DTS(I) will be used, days. (F10.0)

Record 8--Number of Print Intervals (I5)

NPRINT = number of print intervals. (I5)

Record 9--Print Intervals (4(F10.0, F10.0))

PRINT(I) = print interval to be used until time TPRINT(I), days. (F10.0)

TPRINT(I) = time up to when print interval PRINT(I) will be used, days. (F10.0)

Record 10--System Bypass Options (16I5)

SYSBY(K) = bypass option for system K; 0 = system will be simulated; 1 = system will be bypassed. (I5)

2.2 THE EUTROPHICATION MODEL

When running EUTRO5, the number of systems, NOSYS, must be set to 8 or 9 in Record 4. The bypass options in Record 10, SYSBY(K), should be set to 0 for those variables checked in the relevant complexity level in Table 1; they should be set to 1 for those variables not checked in the relevant complexity level in Table 1.

2.3 THE TOXIC CHEMICAL MODEL

When running TOXI5, the number of systems, NOSYS, can be set from 1 to 6 in Record 4, depending upon the solids and kinetic complexity levels chosen for simulation. The bypass options in Record 10, SYSBY(K), should be set to 0 for those variables checked in the relevant complexity level in Table 2; they should be set to 1 for those variables not checked in the relevant complexity level in Table 2.

CHAPTER 3

DATA GROUP B: EXCHANGE COEFFICIENTS

Exchange coefficients for surface water and pore water are computed from input dispersion coefficients, cross-sectional areas, and characteristic lengths. Dispersion coefficients may vary in time according to piecewise-linear time functions, with groups of segment pairs having the same dispersion time function. Exchange data are read for each exchange field. Field one contains dispersion coefficients for water column exchanges. Field two contains exchange data for pore water exchange.

3.1 RECORD FORMATS

Record 1--Number of Exchange Fields (I5, 75X)

NRFLD = number of exchange fields. NRFLD will generally equal 2 for water column and pore water exchanges. (I5)

TITLE = name of data group. (75X)

If no exchange rates are to be read, set NRFLD to zero and continue with Data Group C. If only surface water exchanges are to be read, set NRFLD to 1 and input the proper values in records 2-6 and 12. If pore water exchanges are to be read, set NRFLD to 2 and input the proper values in records 2-12.

Record 2--Exchange Time Functions for Surface Water Field (I5, 2F10.0)

NTEX(1) = number of exchange time functions for field 1. (I5)

SCALR = scale factor for exchange coefficients. All exchange coefficients for field 1 will be multiplied by this factor. (F10.0)

CONVR = conversion factor for exchanges in field 1. (F10.0)

To skip surface water exchange field, set NTEX(1) to zero and continue with the pore water exchange field (record 7) or the exchange bypass options (record 12).

Records 3-6 are input as a group NTEX(1) times:

Record 3--Exchange Data (I5)

NORS(1,NT) = number of exchanges for field 1, time function NT. (I5)

Record 4--Areas, Characteristic Lengths (2F10.0, 2I5)

A(K) = area in square meters for exchange pair K. (F10.0)

EL(K) = characteristic length in meters for exchange pair K. (F10.0)

IR(K),JR(K) = segments between which exchange occurs. The order of the segments is unimportant. (2I5)

Record 4 is repeated NORS(1,NT) times.

Record 5--Number of Breaks in Time Function (I5)

NBRKR(1,NT) = number of values and times used to describe dispersion coefficient piecewise-linear time function. (I5)

Record 6--Piecewise Linear Dispersion Time Function (4(F10.0, F10.0))

RT(K) = value of dispersion coefficient in m^2/sec at time TR(K). (F10.0)

TR(K) = time in days. (F10.0)

Record 6 is repeated NBRKR(1,NT)/4 times.

Record 7--Exchange Time Functions for Pore Water Field (I5, 2F10.0)

NTEX(2) = number of exchange time functions for field 2. (I5)

SCALR = scale factor for exchange coefficients. All exchange coefficients for field 2 will be multiplied by this factor. (F10.0)

CONVR = conversion factor for exchanges in field 2. (F10.0)

To skip pore water exchange field, set NTEX(2) to zero and continue with record 12.

The user should in most situations bypass the exchange for the periphyton/macrophyte system to prevent periphyton or macrophytes from being dispersed since they are anchored to the bottom.

Records 8-11 are input as a group NTEX(2) times:

Record 8--Exchange Data (I5)

NORS(2,NT)	=	number of exchanges for field 2, time function NT. (I5)

NT = 1, NTEX(2)

Record 9--Areas, Characteristic Lengths (2F10.0, 2I5)

A(K)	=	area in square meters for exchange pair K. (F10.0)
EL(K)	=	characteristic length in meters for exchange pair K. (F10.0)
IR(K),JR(K)	=	segments between which exchange occurs. The order of the segments is unimportant. (2I5)

Record 9 is repeated NORS(2,NT) times.

Record 10--Number of Breaks in Time Function (I5)

NBRKR(2,NT)	=	number of values and times used to describe dispersion coefficient piecewise-linear time function. (I5)

Record 11--Piecewise Linear Dispersion Time Function (4(F10.0, F10.0))

RT(K)	=	value of dispersion coefficient in m^2/sec at time TR(K). (F10.0)
TR(K)	=	time in days. (F10.0)

Record 11 is repeated NBRKR(2,NT)/4 times.

Record 12--Exchange Bypass Options (16I5)

RBY(K) = exchange bypass option for system K; 0 = exchange occurs in system K; 1 = bypass exchange for system K. (I5)

K = 1, NOSYS

Record 1 is entered once for Data Group B. Records 2 through 6 are input for the surface water exchange field, with Records 3, 4, 5, and 6 being repeated for each time function in this exchange field. Record 4 uses as many lines as necessary to input NORS sets of A(K), EL(K), IR(K), and JR(K), with 1 set on each line. Record 6 uses as many lines as needed to input NBRKR pairs of RT(K) and TR(K), with 4 pairs occupying each line.

Records 7 through 11 are input for the pore water exchange field, with Records 8, 9, 10, and 11 being repeated for each time function in this exchange field. Record 9 uses as many lines as necessary to input NORS sets of A(K), EL(K), IR(K), and JR(K), with 1 set on each line. Record 11 uses as many lines as needed to input NBRKR pairs of RT(K) and TR(K), with 4 pairs occupying each line.

After data for all exchange fields are entered, Record 12 is input on the following line with NOSYS entries.

CHAPTER 4

DATA GROUP C: VOLUMES

Data Group C is composed of two blocks of data. Initial segment volumes are provided in Data Block C1. In addition, segment type and underlying segment numbers are specified. Hydraulic geometry information can be given to derive segment average depth and velocity as a function of flow. These values are used in reaeration and volatilization calculations only (not in the basic transport calculations.)

The WASP 5.2-MDEP version developed for Maine DEP provides two options for computation of tidal flow based on simple tidal prism flow or depth-time functions in estuarine environments specified by a new flag IDOPT in Record 1 of Data Block C1. Computation of tidal flow based on simple tidal prism or depth-time functions is provided in Data Block C2 as option IDOPT = 1. With this option tidal flows are computed in superposition to any flows specified as flow-time functions in Data Group D. The conversion of depth to flow is based on a user-input segment surface area that is held constant over time. Alternatively, with option IDOPT = 2, segment depth is computed using either a sinusoidal function or a user-specified depth-time function, but flow-time functions are independently specified in Data Group D. The program computes segment bottom area and surface area as the segment volume divided by the segment depth, thus this option allows segment area to vary with time. Time-varying bottom area may be an important feature in sediment oxygen demand and other sediment fluxes in tidal estuaries.

4.1 RECORD FORMATS

DATA BLOCK C1: VOLUMES

Record 1--Preliminary Data (2I5, F10.0, 60X)

IVOPT = water column volume option -- 1 = constant water column volumes; 2, 3 = volumes adjusted to maintain flow continuity. (I5)

IBEDV = benthic volume option -- 0 = constant bed volumes; 1, bed volumes change in response to sediment transport. (I5)

TDINTS = benthic time step in days for recomputing porosity (if IBEDV = 0) or for sediment bed compaction (if IBEDV = 1). (F10.0)

IDOPT = flow option:

0 = Specify flows in Data Group D.
1 = Flow computed by tidal prism or by using depth-time functions assuming constant surface area equal to bottom area.
2 = Depth (but not flow) computed by sinusoidal function or by using depth-time functions. Flow is specified in Data Group D. Bottom area varies as segment volume divided by segment depth. (I5)

TITLE = name of data group. (55X)

Record 2--Scale Factors (2F10.0)

SCALV = scale factor for volumes. All volumes will be multiplied by this factor. (F10.0)

CONVV = conversion factor for volumes. (F10.0)

Record 3 is repeated NOSEG times:

Record 3--Segment Types and Volumes (3I10, 5F10.0)

ISEG = segment number.

IBOTSG = segment immediately below ISEG. (I10)

ITYPE(ISEG) = segment types: 1 = surface water segment, 2 = subsurface water segment, 3 = upper bed segment, 4 = lower bed segment. (I10)

BVOL(ISEG) = volume of segment ISEG in cubic meters. (F10.0)

VMULT(ISEG) = hydraulic coefficient "a" for velocity in ISEG as a function of flow:

$$v = a Q^b$$

If b = 0, VMULT is a constant velocity in m/sec. (F10.0)

VEXP(ISEG) = hydraulic exponent "b" for velocity in ISEG as a function of flow (0-1). A value of 0.4 represents rectangular channels. (F10.0)

DMULT(ISEG) = hydraulic coefficient "c" for depth of ISEG as a function of flow:

$$d = c\,Q^{d}$$

If d = 0, DMULT is a constant depth in m. (F10.0)

DXP(ISEG) = hydraulic exponent "d" for depth of ISEG as a function of flow (0-1). A value of 0.6 represents rectangular channels. (F10.0)

Note that the four hydraulic geometry parameters are used to calculate segment velocity and depth, which are not used by WASP5 in transport calculations. These are used to calculate reaeration or volatilization from segments.

Records 1 and 2 are entered once for Data Group C. Record 3 is repeated NOSEG times. If ICFL = 2 in Data Group A, volumes are read from the restart file (*.RST, where * is the input data set name), and Records 2 and 3 should not be included in the input data set.

DATA BLOCK C2: Computation of Tidal Flow Based on Simple Tidal Prism or Depth-Time Functions

Record 1--Number of Depth-Time Functions

NIND number of depth-time functions. (I5)

SCALD scale factor. (F10.0)

CONVD units conversion factor. (F10.0) (0.3048 for feet to meters)

Records 2 - 5 are input as a group NIND times:

Record 2--Number of Segments for Time Function

NODS(ND) number of unit depth responses for time function ND; each unit response is defined for a single segment. (I5)

Record 3 is repeated NODS(ND) times:

Record 3--Tidal Depth-Time Parameters

ISEGD(ND,K) segment number. (I5)

SAREA(ND,K) surface area of segment ISEGD in square meters. (F10.0) (Not required if IDOPT = 2)

ASEGD(ND,K) amplitude of tidal range at Segment ISEGD in meters. (F10.0) (Required only if NDTYPE(ND) = 1)

TSEGD(ND,K) time lag of tidal range at Segment ISEGD in days. (F10.0) The time lag is used, for example, in case the time of high tide is later at some segments compared to the estuary mouth. (Required only if NDTYPE(ND) = 1)

DSEGD(ND,K) mean water elevation at Segment ISEGD in meters. (F10.0) (Required only if NDTYPE(ND) = 1)

K = 1, NODS(ND)

Record 4--Depth-Time Functions

NDTYPE (ND) = 0, specified depth-time functions
= 1, sinusoidal function. (I5)

NBRKD (ND) for NDTYPE(ND) = 0, number of depths and times used to describe piecewise-linear depth-time function. (I5)

PHASED(ND) for NDTYPE(ND) = 1, phase lag (in days) of sinusoidal depth-time function. The phase lag allows you to vary the tidal stage at the start of a simulation (e.g., high tide or low tide). (F10.0)

PERD(ND) for NDTYPE(ND) = 1, period (in days) of sinusoidal depth-time function (PERD = 0.52 days for a typical semi-diurnal tide). (F10.0)

Record 5 is repeated NBRKD(ND)/4 times and included only if NDTYPE(ND)=0:

Record 5--Piecewise-Linear Depth-Time Function (4(2F10.))
(include only if NDTYPE(ND) = 0 and NBRKD(ND) > 0)

DPT(ND,K) depth (non-dimensional). (F10.0)

TD(ND,K) time in days. (F10.0)

K = 1, NBRKD(ND)

Records 6 and 7 are not included if IDOPT=2:

Record 6--Number of Tidal Segments

NTS	number of tidal segments. (I5)
TITLE	name of data group. (75X)

If included, Record 7 is repeated NTS/20 times:

Record 7--Flow Sequence for Tidal Segments

ITIDE(ITS)	segment numbers of tidal segments in upstream to downstream order (i.e., from head of tide to mouth). (20I5)

ITS = 1, NTS

Record 1 is entered once for Data Block C2. The group of Records 2 through 5 is repeated NIND times (for ND=1,NIND). Records 6 and 7 are not included if IDOPT = 2.

CHAPTER 5

DATA GROUP D: FLOWS

5.1 MODEL TRANSPORT WITH TIDAL FLOWS

WASP5 (version 5.1, 1993) computes volume from the advective flow balance and depth as a function of flow from the exponential hydraulic geometry equations. Bottom area for SOD is implicitly computed as volume divided by depth and is equal to the segment surface area. The computed depth may not accurately reflect the actual depth, nor the computed bottom area the actual bottom area. The new transport representation in WASP 5.2-MDEP is intended to fix this.

WASP 5.2-MDEP provides two options, specified by a new flag IDOPT in Record 1 of Data Block C1. The flag, IDOPT = 0 is the default, which duplicates the WASP5 input options to preserve backward compatibility. With IDOPT = 0, flow must be specified entirely using Data Group D.

The flag, IDOPT = 1 indicates use of available field data or a presumed sinusoidal tidal depth variation to compute flows in estuarine environments based on simple tidal prism calculations. The flag IDOPT = 2 indicates a similar calculation, but for tidal depth only, and not tidal flow. To accommodate these new features, a new Data Block C2 for computation of tidal flow based on simple tidal prism or depth-time functions is included in WASP 5.2-MDEP. The required input for the flag, IDOPT = 1 or 2, is specified using Records 1 through 7 of Data Block C2. An automatic internal calculation of a sinusoidal time variation is also included in WASP 5.2-MDEP. Flows may still be specified under Data Group D even when the tidal flow calculation is specified. In that case, tidal flow volumes are adjusted to account for the flows specified under Data Group D.

WASP 5.2-MDEP computes water-column volume assuming a constant surface area and equal bottom area under IDOPT = 1 under Data Group C. Alternatively, with IDOPT = 2, the program computes bottom area for the SOD and other benthic fluxes using the specified sinusoidal depth variation or depth-time functions with the WASP5 algorithm that bottom area = surface area = volume/depth.

5.2 RECORD FORMATS

Data Group D provides for the advective transport flows that are used in the model. Flows may be input for up to 6 transport fields. Field one consists of advective flows in the water

column. Field two consists of pore water flows. Fields three, four, and five consist of sediment transport velocities and cross-sectional areas for solids. A separate sediment transport field is specified for each of up to 3 solids types. Field six is for evaporation and precipitation velocities and cross-sectional areas. All flows may vary in time according to piecewise linear time functions.

Record 1 is read first. If IQOPT = 1 or 2, Data Block D1 is read next; if IQOPT = 3, Data Block D1 is skipped. Data Blocks D2, D3, D4, D5, and D6 follow in order for NFIELD = 2, 3, 4, 5, and 6, respectively. Following all specified Data Blocks, Record 32 is read.

Record 1--Data Input Options: Number of Flow Fields (2I5, A12)

IQOPT = flow option:

1 = field one (advective) flows are specified directly by user. Individual flows at each segment interface are summed by the model, and the net flow is applied across the interface.

2 = field one flows are specified directly by the user. Individual flows at each segment interface are applied directly by the model.

3 = flows are read from a formatted file created by DYNHYD5 or other hydrodynamic model. (I5)

NFIELD = number of flow fields. The first two fields are surface water and pore water flows. An additional field (3, 4, or 5) is used for each type of solid modeled. Field 6 is used for evaporation and precipitation. If no flows are used, set NFIELD to zero and continue with Data Group E. (I5)

HYDFIL = name of hydrodynamic file to be read by WASP5 during the simulation (for example, RIVER1.HYD). (A12)

DATA BLOCK D1: Direct Input of Field One Flows (IQOPT = 1,2)

Record 2--Number of Flow Time Functions (I5, 2F10.0)

NINQ(1) = number of time functions for Field One. If no flows are used in field one, set NINQ to zero and skip to next field. (I5)

SCALQ = scaling factor. All flows in Field one are multiplied by SCALQ. (F10.0)

CONVQ = units conversion factor. (F10.0)

Records 3 - 6 are input as a group NINQ(1) times:

Record 3--Number of Flows (I5)

NOQS(1,NI) = number of unit flow responses in field one, time function NI; each unit flow is defined for a single segment pair. (I5)

Record 4--Flow Routing for Field One (4(F10.0, 2I15))

BQ(1,NI,K) = portion of flow for field one, time function NI that flows between segment pair K. (F10.0)

JQ(1,NI,K) = upstream segment. (I5)

IQ(1,NI,K) = downstream segment. (I5)

Record 4 is repeated NOQS(1,NI)/4 times.

Record 5--Number of Breaks in Advective Time Functions (I5)

NBRKQ(1,NI) = the number of flows and times used to describe piecewise linear time function NI. (I5)

Record 6--Piecewise Linear Advective Time Function (4(2F10.0))

QT(1,NI,K) = advective flow in m^3/s. (F10.0)

TQ(1,NI,K) = time in days. (F10.0)

Record 6 is repeated NBRKQ(1,NI) times.

Record 2 is input once for Data Block D1. Records 3, 4, 5, and 6 are input once for each flow time function. Record 4 uses as many lines as needed to input NOQS sets of BQ, JQ, and IQ, with four sets per line. Record 6 uses as many lines as

necessary to input NBRKQ sets of QT and TQ, with four sets on each line.

DATA BLOCK D2: Field Two (Pore Water) Flows

Record 7--Number of Pore Water Time Functions (I5, 2F10.0)

NINQ(2) = number of pore water time functions. If no flows are used in Field Two, set NINQ to zero and skip to sediment transport fields. (I5)

SCALQ = scaling factor for pore water flows. (F10.0)

CONVQ = units conversion factor. (F10.0)

Records 8 - 11 are input as a group NINQ(2) times:

Record 8--Number of Flows (I5)

NOQS(2,NI) = number of segment pair flows in Field 2, time function NI. (I5)

Record 9--Flow Routing for Field Two (4(F10.0, 2I5))

BQ(2,NI,K) = portion of pore water flow for time function NI that flows between segment pair K. (F10.0)

JQ(2,NI,K) = upstream segment. (I5)

IQ(2,NI,K) = downstream segment. (I5)

Record 9 is repeated NOQS(2,NI)/4 times.

Record 10--Number of Breaks in Pore Water Time Function (I5)

NBRKQ(2,NI) = number of pore water flows and times used to describe piecewise linear time function NI. (I5)

Record 11--Piecewise Linear Velocity Time Function (4(2F10.0))

QT(2,NI,K) = pore water flow in m^3/s. (F10.0)

TQ(2,NI,K) = time in days. (F10.0)

Record 11 is repeated NBRKQ(2,NI)/4 times.

Record 7 is input once for Data Group D2. Records 8, 9, 10 and 11 are input once for each pore water time function. Record 9 uses as many lines as necessary to input NOQS sets of BQ, JQ, and IQ, with four sets on each line. Record 11 uses as many lines as necessary to input NBRKQ sets of QT and TQ, with four sets on each line.

DATA BLOCK D3: Sediment 1 Transport Field

Sediment transport flow data are input as velocities and areas. Velocities may vary in time, and represent settling, sedimentation, deposition, and scour. Only solids and sorbed chemical are transported by these fields. A separate field is specified for each sediment size fraction. If no solids are modeled, skip directly to Record 32 (Flow Bypass Options).

Record 12--Number of Velocity Time Functions (I5, 2F10.0)

NINQ(3) = number of velocity time functions for Field 3. (I5)

SCALQ = scaling factor for velocities. (F10.0)

CONVQ = units conversion factor. (F10.0)

Records 13 - 16 are input as a group NINQ(3) times:

Record 13--Number of Segment Pairs (I5)

NOQS(3,NI) = number of segment pairs involved in sediment 1 transport. (I5)

Record 14--Areas for Settling, Resuspension (4(F10.0, 2I5))

BQ(3,NI,K) = area in square meters between segment pair K. (F10.0)

JQ(3,NI,K) = segment sediment is transported from. (I5)

IQ(3,NI,K) = segment sediment is transported to. (I5)

Record 14 is repeated NOQS(3,NI)/4 times.

Record 15--Number of Breaks in Velocity Time Function (I5)

NBRKQ(3,NI) = number of velocities and times used to describe piecewise linear time function NI. (I5)

Record 16--Piecewise Linear Velocity Time Function (4(2F10.0))

QT(3,NI,K) = sediment 1 transport velocity in m/day. (F10.0)

TQ(3,NI,K) = time in days. (F10.0)

Record 16 is repeated NBRKQ(3,NI)/4 times.

Record 12 is input once for Data Block D3. Records 13, 14, 15 and 16 are input for each velocity time function. Record 14 uses as many lines as needed to input NOQS sets of BQ, JQ, and IQ, with four sets on one line. Record 16 uses as many lines as needed to input NBRKQ sets of QT and TQ, with four sets per line.

DATA BLOCK D4: Sediment 2 Transport Field

Sediment transport flow data are input as velocities and areas. Velocities may vary in time, and represent settling, sedimentation, deposition, and scour. Only solids and sorbed chemical are transported by these fields. A separate field is specified for each sediment size fraction. If no solids 2 are modeled, enter 0 for NINQ(4), then skip directly to the next data block.

Record 17--Number of Velocity Time Functions (I5, 2F10.0)

NINQ(4) = number of velocity time functions for Field 4. (I5)

SCALQ = scaling factor for velocities. (F10.0)

CONVQ = units conversion factor. (F10.0)

Records 18 - 21 are input as a group NINQ(4) times:

Record 18--Number of Segment Pairs (I5)

NOQS(4,NI) = number of segment pairs involved in sediment 2 transport. (I5)

Record 19--Areas for Settling, Resuspension (4(F10.0, 2I5))

BQ(4,NI,K) = area in square meters between segment pair K. (F10.0)

JQ(4,NI,K) = segment sediment is transported from. (I5)

IQ(4,NI,K) = segment sediment is transported to. (I5)

Record 19 is repeated NOQS(4,NI)/4 times.

Record 20--Number of Breaks in Velocity Time Function (I5)

NBRKQ(4,NI) = number of velocities and times used to describe piecewise linear time function NI. (I5)

Record 21--Piecewise Linear Velocity Time Function (4(2F10.0))

QT(4,NI,K) = sediment 2 transport velocity in m/s. (F10.0)

TQ(4,NI,K) = time in days. (F10.0)

Record 21 is repeated NBRKQ(4,NI)/4 times.

Record 17 is input once for Data Block D4. Records 18, 19, 20 and 21 are input for each velocity time function. Record 19 uses as many lines as needed to input NOQS sets of BQ, JQ, and IQ, with four sets on one line. Record 21 uses as many lines as needed to input NBRKQ sets of QT and TQ, with four sets per line.

DATA BLOCK D.5: Sediment 3 Transport Field

Sediment transport flow data are input as velocities and areas. Velocities may vary in time, and represent settling, sedimentation, deposition, and scour. Only solids and sorbed chemical are transported by these fields. A separate field is specified for each sediment size fraction. If no solids 3 are modeled, enter 0 for NINQ(5), then skip directly to the next data block.

Record 22--Number of Velocity Time Functions (I5, 2F10.0)

NINQ(5) = number of velocity time functions for Field 5. (I5)

SCALQ = scaling factor for velocities. (F10.0)

CONVQ = units conversion factor. (F10.0)

Records 23 - 26 are input as a group NINQ(5) times:

Record 23--Number of Segment Pairs (I5)

NOQS(5,NI) = number of segment pairs involved in sediment 3 transport. (I5)

Record 24--Areas for Settling, Resuspension (4(F10.0, 2I5))

BQ(5,NI,K) = area in square meters between segment pair K. (F10.0)

JQ(5,NI,K) = segment sediment is transported from. (I5)

IQ(5,NI,K) = segment sediment is transported to. (I5)

Record 24 is repeated NOQS(5,NI)/4 times.

Record 25--Number of Breaks in Velocity Time Function (I5)

NBRKQ(5,NI) = number of velocities and times used to describe piecewise linear time function NI. (I5)

Record 26--Piecewise Linear Velocity Time Function (4(2F10.0))

QT(5,NI,K) = sediment 3 transport velocity in m/s. (F10.0)

TQ(5,NI,K) = time in days. (F10.0)

Record 26 is repeated NBRKQ(5,NI)/4 times.

Record 22 is input once for Data Block D5. Records 23, 24, 25 and 26 are input for each velocity time function. Record 24 uses as many lines as needed to input NOQS sets of BQ, JQ, and IQ, with four sets on one line. Record 26 uses as many lines as needed to input NBRKQ sets of QT and TQ, with four sets per line.

DATA BLOCK D6: Evaporation and Precipitation Field

Evaporation and precipitation flow data are input as velocities and areas. Velocities may vary in time to represent rainfall events or seasonal evaporation. No chemical is transported with evaporation, but volumes are adjusted to maintain continuity. If this field is not modeled, skip directly to Record 32 (Flow Bypass Options). After all transport field

data are entered, Record 32 is input with NOSYS entries. If no evaporation or precipitation fields are specified, Record 32 follows Data Group D.5 (solids 3 transport).

Record 27--Number of Velocity Time Functions (I5, 2F10.0))

NINQ(6) = number of velocity time functions for Field 6. (I5)

SCALQ = scaling factor for velocities. (F10.0)

CONVQ = units conversion factor. (F10.0)

Records 28 - 31 are input as a group NINQ(6) times:

Record 28--Number of Segment Pairs (I5)

NOQS(6,NI) = number of segment pairs involved in evaporation or precipitation. (I5)

Record 29--Areas for Evaporation, Precipitation (4(F10.0, 2I5))

BQ(6,NI,K) = area in square meters between segment pair K. (F10.0)

JQ(6,NI,K) = segment water is transported from; if = 0, this is precipitation. (I5)

IQ(6,NI,K) = segment water is transported to; if = 0, this is evaporation. (I5)

Record 29 is repeated NOQS(6,NI)/4 times.

Record 30--Number of Breaks in Velocity Time Function (I5)

NBRKQ(6,NI) = number of velocities and times used to describe piecewise linear time function NI. (I5)

Record 31--Piecewise Linear Velocity Time Function (4(2F10.0))

QT(6,NI,K) = water transport velocity in m/s; if more traditional units of cm/day or cm/year are desired, then specify CONVQ = $1.1574E^{-7}$ or $3.169E^{-10}$, respectively. (F10.0)

TQ(6,NI,K) = time in days. (F10.0)

Record 31 is repeated NBRKQ(6,NI)/4 times.

END OF DATA BLOCKS FOR D

Record 32--Flow Bypass Options (16I5)

QBY(ISYS) = flow bypass option -- 0 = flow transport occurs in system ISYS; 1 = flow transport is bypassed for system ISYS. (I5)

ISYS = 1, NOSYS

The flow bypass option allows flow transport to be set to zero in one or more systems. The bypass option applies to all transport fields.

The user should in most situations bypass the flow calculations for the periphyton/macrophyte system to prevent periphyton and macrophytes from being advected since they are anchored to the bottom.

5.3 THE EXTERNAL HYDRODYNAMIC FILE

When IQOPT in Record 1 is set to 3, external flows and volumes will be read from a formatted ASCII file chosen by the user. This file begins with information on the WASP5 calculational time step, simulation start and end times, and flow connections. The body of the file is composed of sets of segment records and segment interface records that are repeated every time step for the entire simulation. The segment records specify instantaneous segment volumes, depths, and water velocities at the beginning of a time step. The segment interface records specify average interfacial flows during the time step.

WASP5 uses the interfacial flows to calculate mass transport, and the volumes to calculate constituent concentrations. Segment depths and velocities are used only to calculate reaeration or volatilization rates.

Five records comprise the external hydrodynamic file:

Record 1 -- Data Options (2I5, 3F20.0, I5)

NQSEG = Number of segments connected by flows from the hydrodynamic file. (I5)

NQINT = Number of interfacial flow pairs from the hydrodynamic file. (I5)

DELTQ = WASP5 time step; an even multiple of the hydrodynamic time step, seconds. (F20.0)

TBEGIN = Beginning time for the hydrodynamic file, in seconds. (F20.0)

TEND = Ending time for the hydrodynamic file, in seconds. (F20.0)

FILOPT = Switch controlling the contents of the hydrodynamic file; 0 = time variable segment depths and velocities are read; 1 = time variable segment depths and velocities are not read. (I5)

Record 2 -- Segment Interface Pairs (2I5)

IQ(J) = First segment in interface "J", nominally where flow is *from*. (I5)

JQ(J) = Second segment in interface "J", nominally where flow is *to*. (I5)

Note that positive values of flow go from IQ to JQ. Negative values of flow go from JQ to IQ.

Record 2 is repeated NQINT times, for J from 1 to NQINT.

Record 3 -- Initial Segment Properties (4F20.0)

BVOL(I) = Volume of segment "I" at beginning of time step, m^3. (F20.0)

DUMMY = Dummy variable, not used by WASP5. (20.0)

DEPTH(I) = Average depth of segment "I", in meters. (F20.0)

VELOC = Average velocity of segment "I", m/sec. (F20.0)

Record 3 is repeated NQSEG times, for I from 1 to NQSEG.

Records 4 and 5 are repeated as a unit for the number of time steps in the water quality simulation, or (TEND - TBEGIN)/DELTQ:

Record 4 -- Segment Interfacial Flows (F20.0)

BQ(J) = Average flow in interfacial pair "J" during the time step, in m^3/sec. (F20.0)

Record 4 is repeated NQINT times, for J from 1 to NQINT (in the same order as segment pairs are given in Record 2).

Record 5 -- Segment Properties (4F20.0)

BVOL(I) = Volume of segment "I" at end of time step, m^3. (F20.0)

DUMMY = Dummy variable, not used by WASP5. (20.0)

DEPTH(I) = Average depth of segment "I", in meters. (F20.0)

VELOC = Average velocity of segment "I", m/sec. (F20.0)

Record 5 is repeated NQSEG times, for I from 1 to NQSEG.

Record 1 is input once. Record 2 is repeated NQINT times. Record 3 is repeated NQSEG times. Records 4 and 5 are a set, and are repeated (as a set) (TEND - TBEGIN)/DELTQ times. Within each set, Record 4 is repeated NQINT times and Record 5 is repeated NQSEG times.

CHAPTER 6

DATA GROUP E: BOUNDARY CONCENTRATIONS

Data Group E supplies concentrations for each system at the model network boundaries. Model boundaries consist of those segments that import, export, or exchange water with locations outside the network, as specified in Data Groups B and D. All system concentrations from 1 to NOSEG must be supplied for each boundary. Boundary concentrations vary with time following a piecewise linear time function specified by the user in Records 3 and 4.

6.1 RECORD FORMATS

Data Group E is repeated, in its entirety, NOSYS times.

Record 1--Data Input Option--Number of Boundary Conditions (I10, 70X)

NOBC(K) = number of boundary conditions used for system K. (I10)

TITLE = name of data group. (70X)

If no boundary conditions are to be input for system K, set NOBC(K) equal to zero and either continue with the next system or go to Data Group F if K is the last system.

Record 2--Scale Factor for Boundary Conditions (2F10.0)

SCALB = scale factor for boundary conditions. All boundary conditions will be multiplied by this factor. (F10.0)

CONVB = unit conversion factor for boundary conditions. Boundary conditions are expected to be in mg/L (i.e. - g/m^3), in which case CONVB will be 1.0. (F10.0)

Records 3-4 are input as a unit NOBC(K) times:

Record 3--Boundary Location (2I5)

IBC(K) = boundary segment number. (I5)

NOBRK(K) = number of values and times used to describe the broken line approximation. The number of breaks must be equal for all boundary conditions within a system. (I5)

Record 4--Boundary Concentrations (4(2F10.0))

BCT(K) = value of the boundary concentration at time T(K) in mg/L. (F10.0)

T(K) = time in days. If the length of the simulation exceeds T(NOBRK), the broken line approximation is repeated, starting at T(1), i.e., the approximation is assumed to be periodic, with period equation to T(NOBRK). All break times must agree for all segments, i.e., T(1) must be the same for all boundaries, T(2) must be the same for all boundaries, etc. (F10.0)

Record 4 is repeated NOBRK(K)/4 times.

Records 1 and 2 are entered once. Records 3 and 4 are a set and are repeated NOBC times. Within each NOBC set, Record 3 is entered once and Record 4 is repeated until NOBRK entries are input. Four entries (four BCT(K)-T(K) pairs) will fit on each 80-space line. The whole group (Records 1 - 4) is repeated NOSYS times, once for each model system.

6.2 THE EUTROPHICATION MODEL

When running EUTRO5, Data Group E is input 9 times, once for each system. For those systems being bypassed, the user may specify 0 for the number of boundary conditions, and skip to the next system.

The user should be careful to note that boundary concentrations for system 4, phytoplankton, are input as chlorophyll a, in μg/L. These are transformed internally to phytoplankton carbon using the carbon to chlorophyll ratio, which is specified in Data Group H as constant 46.

6.3 THE TOXIC CHEMICAL MODEL

When running TOXI5, Data Group E is input NOSYS times, once for each system simulated. NOSYS is specified in Data Group A, and has a maximum value of 6. For those systems being bypassed, the user may specify 0 for the number of boundary conditions, and skip to the next system.

The user should be careful to note that all boundary concentrations are input in the standard WASP units of mg/L (even though the output concentrations for chemical are in units of μg/L.)

CHAPTER 7

DATA GROUP F: WASTE LOADS

Data Group F is composed of three blocks of data. Data Block F1 contains the point source waste loads used in the model. These loads vary with time following a piecewise linear time function specified by the user in Records 3 and 4. Following complete specification of point source loads, nonpoint source loads are read from Data Block F2, which is composed of only one record in the input dataset. Nonpoint source (NPS) loads vary with time in a daily step function read from an external loading file.

WASP 5.2-MDEP includes an additional Data Block F3, which provides an alternative input option for input of steady NPS loads. Steady NPS loads are expressed in terms of mass load in units such as kilograms per day. The necessary input data structure is accommodated by a change to Record 5 of Data Block F1 and the addition of Data Block F3.

7.1 RECORD FORMATS

Data Block F1 (records 1-4) is repeated in its entirety NOSYS times:

Record 1--Number of Point Source Loadings (I10, 70X)

NOWK(ISYS) = number of point source loadings used for system ISYS. Loadings may also be considered as sources (loads) or sinks of a water quality constituent. If no loadings are to be input, set NOWK(ISYS) to zero, and continue with next system or go to next data group.(I10)

TITLE = name of data group. (70X)

If no point source loadings are to be input for system ISYS, set NOWK(ISYS) equal to zero and either continue with the next system or go to Data Group G if ISYS is the last system.

Record 2--Scale Factor for Point Source Loadings (2F10.0)

SCALW = scale factor for point source loadings. All loadings for system ISYS will be multiplied by this factor. (F10.0)

CONVW = unit conversion factor for point source loadings for system ISYS. Loadings are expected to be in kilograms per day. If loadings are given in English units (pounds per day), this factor will be 0.4535. (F10.0)

Records 3-4 are input as a unit NOWK(ISYS) times:

Record 3--Number of Point Sources (2I5)

IWK(K) = segment number that has point source loading BWK(K). (I5)

NOBRK(K) = number of breaks used to describe the loading function approximation. The number of breaks must be equal for all forcing functions within a system. (I5)

Record 4--Point Source Time Function (4(2F10.0))

WKT(K) = value of the point source loading at time T(K), in kg/day. (F10.0)

T(K) = time in days. If the length of the simulation exceeds T(NOBRK), the approximation is repeated, starting at T(1), i.e., the approximation is assumed to be periodic with period equal to T(NOBRK). All break times must agree for all segments; i.e., T(1) must be the same for all loads, T(2) must be the same for all loads, etc. (F10.0)

Record 4 is repeated NOBRK(ISYS)/4 times.

Records 1 and 2 are input once. Records 3 and 4 are a set and are repeated (as a set) NOWK times. Within each set, Record 3 is entered once and Record 4 is repeated until all NOBRK entries are entered. Four entries (WKT(K)-T(K) pairs) will fit on each 80-space line. The entire group (Records 1 - 4) is repeated NOSYS times, once for each system.

Data Block F2, record 5, is input once:

Record 5--Nonpoint Source Load Option (I10)

LOPT = nonpoint source load option; a value of 0 means that no nonpoint sources will be read from an external file; a value of 1 will cause the model to read a set of loads from an external file; a value of 2 will cause the model to read a set of steady loads from Data Block F3. For LOPT = 1, the user will be prompted by WASP5 to provide information on the external file. This file and its contents are described below. (I10)

Data Block F3: Steady Nonpoint Source (NPS) Waste Loads

Record 1--Number of Steady Runoff Loads (I5,75X)

NOWKS Number of constant nonpoint source loads. A 'load' here means a source of nonpoint source runoff to a single segment, which may carry loads of more than one WASP system. (I5)

TITLE name of data group. (75X)

Record 2--Scaling Factors (10X,7F10.0)

TITLE 10-character identification field so that scaling and conversion factors will line up vertically with loads in Record 4. (10X)

SCALN(K) K = 1, NOSYS. Scale factors for runoff loads for all systems K=1 to NOSYS. All runoff loads will be multiplied by this factor. (7F10.0)

Record 3--Conversion Factors (10X,7F10.0)

TITLE 10-character identification field so that scaling and conversion factors will line up vertically with loads in Record 4. (10X)

CONVN(K), K = 1, NOSYS. Units conversion factors for runoff loads for all systems K=1 to NOSYS. Runoff loads are expected in kilograms per day. If runoff loads are given in English units (pounds per day), this factor will be 0.4535. (7F10.0)

Record 4--Loading Segments and Loads (I5,5X,7F10.0,(10X,7F10.0))

INPS(I) segment number receiving constant nonpoint source load I. (I5,5X)

NPSWK(K,I), K = 1, NOSYS. Segment load for loading segment I and system K. If there are more than 7 systems, system 8 starts in a second record in columns 11-20 (i.e., lined up below that for system 1). (7F10.0)

Record 4 is repeated for NOWKS times (for I=1, NOWKS).

7.2 THE EXTERNAL NONPOINT SOURCE FILE

When LOPT is set to 1, external nonpoint sources will be read from a formatted ASCII file chosen by the user. This file contains information on which WASP5 systems and segments receive nonpoint source loads, and a record of the nonzero loads by system, segment, and day.

Six records comprise the nonpoint source file.

Record 1--Data Options (A15, 3I5)

NPSMOD = Name or description of nonpoint source model or method of generation; this is echoed to the output file for the record. (A15)

NUMSEG = Number of segments receiving nonpoint source loads. (I5)

INTOPT = Interpolation option; 1 = step function (only one in code now). (I5)

NUMSYS = Number of WASP systems receiving nonpoint source loads. (I5)

Record 2--Loading Segments (I5)

LSEG(I) = segment number receiving loads. (I5)

Record 2 is repeated NUMSEG times.

Record 3--Loading Systems (20I5)

LSYS(I) = WASP system numbers receiving loads. (I5)

Record 4--System Descriptors (A15)

NAMESY(I) = Name or description of WASP systems receiving loads. (A15)

Record 4 is repeated NUMSYS times.

Records 5 and 6 are repeated as a unit for the number of days that nonzero loads occur:

Record 5--Loading Days (F10.0)

LDAY = Time in days for the following nonzero load. (F10.0)

Record 6--Nonpoint Source Loads (A15, 20F10.0)

NAMESY(I) = System name or description (not read in by WASP). (A15)

NPSWK(I,J) = Nonpoint source loads for WASP system "I" at all loading segments "J", in the order presented in Record 2. Loads are in kg/day. (20F10.0)

Record 6 is repeated NUMSYS times.

Record 1 is input once. Record 2 is repeated NUMSEG times. Record 3 is then input once. Record 4 is repeated NUMSYS times. Records 5 and 6 are a set and are repeated (as a set) NUMSYS times. Within each set, Record 5 is entered once and Record 6 is repeated NUMSYS times.

7.3 THE EUTROPHICATION MODEL

When running EUTRO5, Data Block F1 is input 8 times, once for each system. For those systems being bypassed, the user may specify 0 for the number of waste loads, and skip to the next system.

The user should note that waste loads for system 4, phytoplankton, are input as phytoplankton carbon, in kg/day.

7.4 THE TOXIC CHEMICAL MODEL

When running TOXI5, Data Block F1 is input NOSYS times, once for each system simulated. NOSYS is specified in Data Group A, and has a maximum value of 6. For those systems being bypassed, the user may specify 0 for the number of waste loads, and skip to the next system.

CHAPTER 8

DATA GROUP G: PARAMETERS

Parameters are spatially-variable characteristics of the water body. The definition of the parameters will vary, depending upon the structure and kinetics of the systems comprising each model. The input format, however, is constant. The number of parameters that is specified in Record 1 must be input for each segment.

WASP 5.2-MDEP has thirteen additional parameters available for EUTRO5 simulations. WASP 5.2 allows algal growth rate, algal respiration rate, algal die-off rate, zooplankton grazing rate, nitrogenous BOD decay rate, and carbonaceous BOD decay rate constants to vary by reach. Card Group H can alternatively be used to specify these constant(s) at once for all segments. Thus, the user has two options for specifying these inputs: for constants that are constant over the entire model domain, Card Group H can be used just as is done in WASP5. For constants that are varied by reach, Card Group G would be used instead. Specifying constants in both Card Groups G and H triggers an error message.

8.1 RECORD FORMATS

Record 1--Number of Parameters (I10, 70X)

NOPAM	=	number of parameters required by the model. If no parameters are to be input, set NOPAM to zero and go to Data Group H. (I10)
TITLE	=	name of data group. (70X)

Record 2--Scale Factors for Parameters (4(A5, I5, F10.0))

ANAME(ISC)	=	descriptive name for parameter ISC. (A5)
ISC	=	parameter number identifying parameter. (I5)
PSCAL(ISC)	=	scale factor for parameter ISC. (F10.0)

Record 2 is repeated NOPAM/4 times.

Records 3-4 are input as a unit NOSEG times:

Record 3--Segment Number (I10)

ISG = segment number for the following parameter values. (I10)

Record 4--Segment Parameters (4(A5, I5, F10.0))

PNAME(ISC) = an optional one to five alphanumeric character descriptive name for parameter PARAM(ISG,ISC). (A5)

ISC = parameter number identifying parameter. (I5)

PARAM(ISEG,ISC)= the value of parameter ISC in segment ISG. (F10.0)

Record 4 is repeated NOPAM/4 times.

Record 1 is input once in Data Group G, occupying one line. Record 2 has NOPAM entries. Four entries will fit on one line; thus, Record 2 uses as many 80-space lines as needed to enter all NOPAM entries. Records 3 and 4 are repeated NOSEG times, once for each segment. For each segment, Record 4 uses as many lines as needed to enter all NOPAM entries.

8.2 THE EUTROPHICATION MODEL

Listed below are the 25 parameters available for EUTRO5 simulations. Six representative levels of analysis were outlined in Table 1. For Level 1 and 2 analyses, only TMPSG, TMPFN, SOD1D, and SODTA (3, 4, 9, and 11) need be specified. Spatially-variable reaeration rate constants may be directly specified using REARSG (14). For Level 3 analysis, VELFN, FNH4, and TOTLIM (1, 7, and 13) may be added (DEPTH, VELFN, and TOTLIM are used to compute reaeration; if rate constant K2 is specified (Constant 82), then VELFN, REARSG, and TOTLIM can be omitted; if parameter REARSG is specified, then VELFN and TOTLIM can be omitted). For analyses at Level 4 and above, all parameters should be considered.

8.2.1 REACH-VARIABLE CONSTANTS

The WASP 5.2-MDEP modifies the approach of WASP 5.1 by allowing the user to vary some of the model constants by reach. However, WASP 5.2-MDEP preserves backward compatibility with prior input data files. Card Group H can be used to specify constant(s) at once for all segments, but WASP 5.2-MDEP also provides the user with the alternative of specifying new reach-

variable constants in Card Group G, wherein they would be allowed to vary by segment. Thus, the user has two options for specifying these inputs: for constants that are constant over the entire model domain, Card Group H would be used just as is done in WASP5. For constants that are varied by reach, Card Group G would be used instead. Specifying constants in both Card Groups G and H would trigger an error message.

In WASP 5.2-MDEP, the following constants are allowed to vary by reach: algal growth rate, algal respiration rate, algal die-off rate, zooplankton grazing rate, nitrogenous BOD decay rate, and carbonaceous BOD decay rate. This list does not translate one-to-one into the constants that are specified in Card Group H for the eutrophication model. The following constants are included as reach-variable constants:

11	K12C	Nitrification rate at 20°C, per day.
13	KNIT	Half-saturation constant for nitrification-oxygen limitation, mg O_2/L.
21	K20C	Denitrification rate at 20°C, per day.
23	KNO3	Half-saturation constant for denitrification oxygen limitation, mgO_2/L.
41	K1C	Saturated growth rate of phytoplankton (day^{-1}).
49	KMPG1	Phosphorous half-saturation constant for phytoplankton growth, mg PO_4-P/L.
50	K1RC	Endogenous respiration rate of phytoplankton at 20°C, day^{-1}.
52	K1D	Non-predatory phytoplankton death rate, day^{-1}.
53	K1G	Grazing rate on phytoplankton per unit zooplankton population, L/cell-day.
71	KDC	CBOD deoxygenation rate at 20 C, per day.
75	KBOD	Half saturation constant for carbonaceous deoxygenation oxygen limitation.
91	K71C	Mineralization rate of dissolved organic nitrogen, per day.
100	K83C	Mineralization rate of dissolved organic phosphorus, per day.

The user is able to read these reach-variable constants in either Card Group G or H depending upon whether they are to be treated as reach-variable or constant throughout the model, respectively.

8.2.2 BENTHIC SOURCE FOR CBOD

There is a lack of symmetry in WASP5 in that in water-column-only models, the code allows fluxes of ammonia and phosphate as well as SOD to be specified, but not CBOD. Similarly, in models with both water column and sediment compartments, fluxes of ammonia, nitrate, phosphorus, and oxygen (as SOD) are calculated, but not CBOD. WASP 5.2-MDEP allows fluxes of CBOD as a remedy.

The equation for carbonaceous oxygen demand in the WASP5 model accounts for input due to death of algae, and loss by oxidation, settling, and denitrification. WASP 5.2-MDEP accounts for input due to death of macrophytes through the addition of a submodel for macrophytes. WASP 5.2-MDEP also accounts for input from CBOD released from the sediment. The variables for CBOD are defined as TFBOD and FBOD:

Benthic CBOD Flux, mg/m^2-day-- The segment- and time-variable benthic BOD flux can be specified using parameter FBOD and time function TFBOD. The product of the spatially-variable FBOD and time-variable TFBOD gives the segment and time specific benthic flux for BOD used by EUTRO5. Flux versus time values can be entered using TFBOD, while unitless segment ratios can be entered using FBOD. Values should be entered for water column segments that are in contact with the bottom of the water body. (Group G, Record 4, PARAM(I,35); Group I, Record 2, VALT(14,K))

Adding this process requires adding a 35th variable onto the PARAM array which is read through the Data Group G input. The additional time function, TBOD, is added to the inputs for Data Group I.

The complete list of parameters is as follows:

ISC	ANAME	Definition and Units
1	VELFN	Pointer to the time-variable velocity function to be used for ISEG. The four velocity functions are defined by the user in data group I.
2	SAL	Average salinity of ISEG, in g/L; used in calculation of DO saturation. This parameter is to

		be omitted if salinity state variable (System 9) is used.
3	TMPSG	Segment temperature multiplier (CC). TMPSG varies over space and can be either actual temperature or a normalized function, depending on the definition of TEMP. TMPSG(ISEG) * TEMP(TMPFN(ISEG)) = STP, the temperature of segment ISEG.
4	TMPFN	Flag designating the time-variable temperature function to be used for ISEG. The four temperature functions are defined by the user in data group I.
5	KESG	Segment extinction coefficient multiplier (m^{-1}). KESG varies over space and can be either an actual extinction coefficient or a normalized function, depending on the definition of KE. KESG(ISEG) * KE(KEFN(ISEG)) = Ke, the extinction coefficient for segment ISEG.
6	KEFN	Pointer designating the time variable extinction coefficient (KE) to be used for segment ISEG. The five extinction coefficients available are defined in data group I.
7	FNH4	Average ammonium flux multiplier for segment (mg/m^2-day).
8	FPO4	Average phosphate flux multiplier for segment (mg/m^2-day).
9	SOD1D	Sediment oxygen demand for segment (g/m^2-day).
10-11	RLGHTS	Used internally; not specified by the user.
12	SODTA	Segment specific temperature correction coefficient (theta) for sediment oxygen demand.
13	TOTLIM	Segment specific percent shading.
14	REARSG	Segment specific reaeration rate constant multiplier, used in combination with time function REAR.
15 to 21		Used internally; not specified by the user.
22	K12C	Nitrification rate at 20°C, per day. (Corresponds to Data Group H constant 11.)

23	KNIT	Half-saturation constant for nitrification-oxygen limitation, mg O_2/L. (Corresponds to Data Group H constant 13.)
24	K20C	Denitrification rate at 20°C, per day. (Corresponds to Data Group H constant 21.)
25	KNO3	Half-saturation constant for denitrification oxygen limitation, mgO_2/L. (Corresponds to Data Group H constant 23.)
26	K1C	Saturated growth rate of phytoplankton (day^{-1}). (Corresponds to Data Group H constant 41.)
27	KMPG1	Phosphorous half-saturation constant for phytoplankton growth, mg PO_4-P/L. (Corresponds to Data Group H constant 49.)
28	K1RC	Endogenous respiration rate of phytoplankton at 20°C, day^{-1}. (Corresponds to Data Group H constant 50.)
29	K1D	Non-predatory phytoplankton death rate, day^{-1}. (Corresponds to Data Group H constant 52.)
30	K1G	Grazing rate on phytoplankton per unit zooplankton population, L/cell-day. (Corresponds to Data Group H constant 53.)
31	KDC	CBOD deoxygenation rate at 20°C, per day. Corresponds to Data Group H constant 71.)
32	KBOD	Half saturation constant for carbonaceous deoxygenation oxygen limitation. (Corresponds to Data Group H constant 75.)
33	K71C	Mineralization rate of dissolved organic nitrogen, per day. (Corresponds to Data Group H constant 91.)
34	K83C	Mineralization rate of dissolved organic phosphorus, per day. (Corresponds to Data Group H constant 100.)
35	FBOD	Average CBOD flux multiplier for segment (mg/m^2-day).

36 SUBFRAC Fraction of bottom available as periphyton substrate, f_A.

8.3 THE TOXIC CHEMICAL MODEL

Listed below are the 18 parameters that may be used by TOXI5. The user need input only those required to model the particular reactions being considered. For solids, equilibrium, and kinetics Level 1, no parameters are necessary.

ISC	ANAME	Definition, Units, and Reactions Affected
1	VELFN	Pointer to water velocity time function (1-4); V.
2	TMPFN	Pointer to normalized temperature time function (1-4); ALL.
3	TEMP	Multiplier for water temperature time function (˚C); ALL.
4	WVEL	Multiplier for wind velocity (10 meters above segment surface) time function (meters/sec); V.
5	REAR	Multiplier of time function 5, whose definition depends on volatilization option XV (constants 236,736,1336): XV = 1 volatilization rate constant (m/day) XV = 2,3 oxygen reaeration rate constant (m/day) XV = 4,5 REAER not used; enter 0; V.
6	DOC	Dissolved organic carbon concentrations (mg/L); S, P.
7	FOC 1	Fraction organic carbon of solids class 1; S.
8	FOC 2	Fraction organic carbon of solids class 2; S.
9	FOC 3	Fraction organic carbon of solids class 3; S.
10	CHPHL	Multiplier for phytoplankton chlorophyll concentration time function (mg/L); P.
11	PH	Multiplier for pH time function; H, I.
12	XKE2	Light extinction coefficient for photochemically active light (1/meter); this value is used only for photolysis option XPHOTO = 2 (constants 286,886,1486). For photolysis option 1 or 2 when XKE2 = 0.0 the extinction coefficient is calculated from solids, DOC, and chlorophyll concentrations; P.

ISC	ANAME	Definition, Units, and Reactions Affected
13	OXRAD	Concentration of oxidants, such as O_3 for H_2O_2 (moles/L); O.
14	BAC	Density of active bacteria (cells/100 cc) the units for bacterial density must be consistent with those used for the second order biodegradation rate constants KBIO20 (constants 146-160, 746-760, 1346-1360); the product of BAC and KBIO20 must be units of day^{-1}; B.
15	EXENV	Property of aquatic environment that affects the user-defined "extra reaction." The units for EXENV must be consistent with those used for second order rate constants KE20 (constant 576-590, 1176-1190, 1776-1790); the product of EXENV and KE20 must yield units of day^{-1}; E.
16	TOTKG 1	Total lumped first-order decay rate constant for chemical 1 in segment (day^{-1}).
17	TOTKG 2	Total lumped first-order decay rate constant for chemical 2 in segment (day^{-1}).
18	TOTKG 3	Total lumped first-order decay rate for chemical 3 in segment (day^{-1}).

I = ionization, S = sorption, V = volatilization, B = biodegradation, H = hydrolysis, O = oxidation, P = photolysis, E = extra reaction

For equilibrium level 2, FOC 1 is used to enter partition coefficients. For equilibrium levels 3 and above, FOC 1 is fraction organic carbon of solids class 1. DOC may be entered. If two or three solids classes are being simulated (solids level 4), then FOC 2 and FOC 3 must be entered. For equilibrium level 5, PH values are necessary.

At kinetics level 2, TOTKG 1 is specified. If two or three chemicals are being simulated at this level, then TOTKG 2 and TOTKG 3 must be specified. Kinetics level 3 may require the remaining parameters, depending on the kinetic processes of importance. If water temperatures differ significantly from 20°C, then TEMP may be necessary for all processes (depending on the accuracy required of the simulation). Volatilization requires REAR for options 1, 2, and 3, but not for 4 and 5. If reareation values are not available for volatilization options 2 and 3, then rates can be calculated internally if parameters DEPTH and VELOC are given. Volatilization options 4 and 5 require parameter WVEL.

Photolysis requires DEPTH values. In addition photolysis option 1 requires DOC and CHPHL. Photolysis option 2 may use either DOC and CHPHL values or XKE2 values. The remaining processes of hydrolysis, oxidation, biodegradation, and extra reaction require one parameter each: PH, OXRAD, BAC, and EXENV, respectively.

CHAPTER 9

DATA GROUP H: CONSTANTS

The definition of the constants will vary, depending upon the structure and kinetics of the systems comprising each model. This data group is subdivided into global constants and constants for each system (thus NOSYS+1 groups are read). Each of these groups can be subdivided into any number of fields containing similar kinds of data.

9.1 RECORD FORMATS

Record 1--Header (80X)

TITLE = name of data group. (80X)

Records 2-4 are input as a group NOSYS+1 times:

Record 2--Data Fields in Group ISYS (A10, I10)

CHNAME(ISYS) = a ten-character descriptive name for System (ISYS). (A10)

NFLD = number of fields of constants for this group; 0 = no constants for this group; the user may subdivide the constants into any number of arbitrary fields. (I10)

If no constants are to be input for this group, set NFLD equal to zero and continue with next group. Records 3 and 4 are repeated as a unit NFLD times.

Record 3--Number of Constants in Field (A10, I10)

FLDNAME = ten-character name identifying field of constants. (A10)

NCONS = number of constants to be entered in this field; 0 = no constants for this field (skip to next field). (I10)

Record 4--Constants (2(A10, I10, F10.0))

TNAME(ISC) = name identifying constant ISC. (A10)

ISC = number identifying constant; these numbers are set by model developer. (I10)

CONST(ISC) = value of constant ISC. (F10.0)

Record 4 is repeated NCONS/2 times.

Record 1 is entered once in Data Group H. Records 2 through 4 are entered as NOSYS + 1 groups. For each group, Records 3 and 4 are entered NFLD times. For each field, Record 4 uses as many lines as needed for NCONS entries (2 per line).

9.2 CALCULATION OF LIGHT INTENSITY

Estimation of solar radiation may be performed using WASP5.2-MDEP as is done in QUAL2 (Brown and Barnwell, 1987) by setting the LGHTS constant in Data Group H (ISC=43) to a negative value. In WASP5, the absolute value of LGHTS is used to designate whether the Smith or DiToro algorithm is used to determine the impact of light on phytoplankton growth. The LGHTS constant is therefore used as follows:

	DiToro	Smith
Input light intensity	1	2
Calculate light intensity	-1	-2

In WASP5.2-MDEP, cloudiness is entered as a time varying function in the climate data file as described below. The remainder of the terms are computed as functions of the site latitude, longitude, and elevation, the dust attenuation factor, the wet-bulb and dry-bulb temperatures, and the local barometric pressure. The temperature and pressure terms are time-varying functions, while the others are constants entered as part of Data Group H. The new constants entered with Data Group H, their ISC numbers and references to their use in the QUAL2 User's Manual are shown below:

ISC	ANAME	Definition and Units
60	LAT	Site latitude, degrees
61	LLM	Longitude of local meridian, degrees

62	LSM	Longitude of standard meridian, degrees
63	ELEV	Site elevation, feet, MSL
65	DAT	Dust attenuation factor (0.0 to 0.13 according to Brown and Barnwell, 1987). Default value = 0.0.
66	TFACT	Fraction of solar radiation that is photosynthetically active. Default value is 0.44.

The following climate time functions are read from the file *climate.dat*:

Definition and Units	Reference in QUAL2 User's Manual
Cloudiness, decimal fraction	Eq. IV-26 on pg. 65
Wet bulb temperature, °F	Eq. IV-34 on pg. 68
Dry bulb temperature, °F	Eq. IV-34 on pg. 68
Local barometric pressure, inches Hg	Eq. IV-34 on pg. 68

Each record in the file *climate.dat* contains a single value of each of these time functions at a specified date and hour. The record format used in QUAL2 has been preserved, so as to make use of available QUAL2 input files. The records are read free format, so that strict columnar formatting is not necessary.

The record contains a year field; however WASP does not make use of this field. Multi-year simulations therefore cannot be run. The climate data functions will not repeat once the simulation has gone beyond the time range over which the function was defined.

The following is sample data from the *climate.dat* file:

Mo	Dy	Yr	Hr	Cloudiness	Wet	Dry	Local
07	01	90	1.	0.57	63.0	54.4	27.46
07	01	90	4.	0.70	59.7	54.3	27.46
07	01	90	7.	0.80	66.0	56.4	27.49

The fields are, from left to right, the month, day, year, hour, cloudiness, wet bulb temperature, dry bulb temperature, and local barometric pressure in units as designated above.

9.3 THE EUTROPHICATION MODEL

Listed below are the 65 constants available for a full eutrophication simulation in WASP 5.2-MDEP. For Maine DEP, eighteen additional constants were added for macrophyte/ periphyton simulation and five additional constants were added for calculation of light intensity. Chapters 4 and 5 discuss the constants required for each level of complexity in dissolved oxygen and eutrophication modeling. Default values for constants are 0 unless otherwise noted.

ISC	ANAME	Definition and Units
11	K12C	Nitrification rate at 20°C, per day.
12	K12T	Temperature coefficient for K1320C. Default = 1.0.
13	KNIT	Half-saturation constant for nitrification-oxygen limitation, mg O_2/L.
21	K20C	Denitrification rate at 20°C, per day.
22	K20T	Temperature coefficient for K140C. Default = 1.0.
23	KNO3	Half-saturation constant for denitrification oxygen limitation, mgO_2/L.
41	K1C	Saturated growth rate of phytoplankton (day^{-1}).
42	K1T	Temperature coefficient. Default = 1.0.
43	LGHTSW	Light formulation switch: LGHTSW = 1, use Di Toro et al. (1971) formulation; LGHTSW = 2, use Dick Smith's (USGS) formulation. Default = 1.
44	PHIMX	Maximum quantum yield constant. Used only when LGHTS = 2, mg C/mole photons. Default = 720.
45	XKC	Chlorophyll extinction coefficient. Used only when LGHTSW = 2, (mg chl**a**/m^3)$^{-1}$/m. Default = 0.017.
46	CCHL	Carbon-to-chlorophyll ratio. Used only when LGHTSW = 1 (mg carbon/mg chl **a**). Default = 30.

47 IS1 Saturation light intensity for phytoplankton. Used only when LGHTSW = 1 (Ly/day). Default = 300.

48 KMNG1 Nitrogen half-saturation constant for nitrogen for phytoplankton growth, which also affects ammonia preference, mg-N/L. NOTE: This affects ammonia preference:

= 0, PNH3G1 = 1.0
= Large, PNH3G1 = $NH_3/(NH_3 + NO_3)$

NOTE: For standard model application, use a large KMNG1.

49 KMPG1 Phosphorous half-saturation constant for phytoplankton growth, mg PO_4-P/L.

50 K1RC Endogenous respiration rate of phytoplankton at 20°C, day^{-1}.

51 K1RT Temperature coefficient for phytoplankton respiration. Default = 1.0.

52 K1D Non-predatory phytoplankton death rate, day^{-1}.

53 K1G Grazing rate on phytoplankton per unit zooplankton population, L/cell-day.

54 NUTLIM Nutrient limitation option. 0 = minimum; 1 = multiplicative. Default = 0.

55 KPZDC Decomposition rate constant for phytoplankton in the sediment at 20°C, per day.

56 KPZDT Temperature coefficient for decomposition of phytoplankton in sediment. Default = 1.0.

57 PCRB Phosphorus-to-carbon ratio in phytoplankton, mg P/mg C. Default = 0.025.

58 NCRB Nitrogen-to-carbon ratio in phytoplankton, mg N/mg C. Default = 0.25.

59 KMPHY Half-saturation constant for phytoplankton, mg carbon/L. NOTE: As phytoplankton concentrations increase, mineralization rates for organic nitrogen and organic phosphorus increase. If KMPHY is small, there is little phytoplankton effect on mineralization. If KMPHY is large, a large concentration of phytoplankton is needed to

		drive mineralization. For standard model application, use KMPHYT = 0.
60	LAT	Site latitude, degrees
61	LLM	Longitude of local meridian, degrees
62	LSM	Longitude of standard meridian, degrees
63	ELEV	Site elevation, feet, MSL
65	DAT	Dust attenuation coefficient (typical value is 0 to 0.13 according to QUAL2 user's manual, Brown and Barnwell, 1987). Default = 0.0.
66	TFACT	Fraction of solar radiation that is photosynthetically active (typical value is 0.43 to 0.45 according to QUAL2 user's manual, Brown and Barnwell, 1987). Default = 0.44
71	KDC	CBOD deoxygenation rate at 20°C, per day.
72	KDT	Temperature coefficient for carbonaceous deoxygenation in water column. Default = 1.0.
73	KDSC	Decomposition rate of carbonaceous BOD in the sediment at 20°C, per day.
74	KDST	Temperature coefficient for carbonaceous deoxygenation in the sediment. Default = 1.0.
75	KBOD	Half saturation constant for carbonaceous deoxygenation oxygen limitation.
81	OCRB	Oxygen to carbon ratio in phytoplankton, mg O_2/mg C. Default = 32/12.
82	K2	Reaeration rate constant at 20°C for entire water body, day^{-1}. NOTE: If K2 is not entered, the reaeration rate will be calculated as the product of parameter REARSG and time function REAR. If parameter REARSG is not entered, the reaeration rate will be calculated from water velocity, depth, and wind velocity.
91	K71C	Mineralization rate of dissolved organic nitrogen, per day.
92	K71T	Temperature coefficient for K1013C. Default = 1.0.

93	KONDC	Decomposition rate constant for organic nitrogen in the sediment at 20°C, per day.
94	KONDT	Temperature coefficient for decomposition of organic nitrogen in the sediment. Default = 1.0.
95	FON	Fraction of dead and respired phytoplankton nitrogen recycled to organic nitrogen. Default = 1.0.
100	K83C	Mineralization rate of dissolved organic phosphorus, per day.
101	K83T	Temperature coefficient for K58C. Default = 1.0.
102	KOPDC	Decomposition rate of organic phosphorus in the sediment at 20°C, per day.
103	KOPDT	Temperature coefficient for decomposition of organic phosphorus in the sediment. Default = 1.0.
104	FOP	Fraction of dead and respired phytoplankton phosphorus recycled to organic phosphorus. Default = 1.0.
105	K2C	Maximum growth rate for periphyton, K_{2c}.
106	K2T	Temperature coefficient for periphyton growth.
107	KMNG2	Half-saturation constant for periphyton for nitrogen, K_{2mN}.
108	KMPG2	Half-saturation constant for periphyton for phosphorus, K_{2mP}.
109	K2RC	Endogenous respiration rate for periphyton, k_{2R}.
110	K2RT	Temperature coefficient for respiration for periphyton.
111	K2DC	Death and grazing rate for periphyton, k_{2D}.
112	K2DT	Temperature coefficient for death and grazing for periphyton.
113	IS2	Saturation light intensity for periphyton. Used only when LGHTSW = 1 (Ly/day). Default = IS1.
114	PCRB2	Phosphorus to carbon ratio for periphyton, a_{2PC}.

115	KMDG2	Half-saturation constant for periphyton for periphyton density, K_{2mD} (mg/m^2). Default = 20.
116	F2OP	Fraction of dead and respired periphyton recycled… to the organic phosphorus pool, f_{2op}.
117	NCRB2	Nitrogen to carbon ratio for periphyton, a_{2NC} .
118	F2ON	Fraction of dead and respired periphyton recycled to the organic nitrogen pool, f_{2ON}.
119	NUTLIM2	Nutrient limitation option for periphyton, 0 = minimum, 1 = multiplicative.
120	KPZDC2	Decomposition rate constant for periphyton in the sediment, k_{PZD2}.
121	KPZDT2	Temperature coefficient for decomposition of periphyton in the sediment.
122	OCRB2	Oxygen to carbon ratio for periphyton, a_{2OC}.
123	F2WC	Fraction of dead periphyton that enters the water column. The fraction (1-F2WC) goes to the underlying sediment segment (if any). Default value = 0.0.

9.4 THE TOXIC CHEMICAL MODEL

A large number of constants are available to characterize the various chemical reactions at different levels of complexity. Very few need be specified for any one simulation. Table 3 summarizes the constants that may be used for equilibrium and kinetics level 1. Only two of these need be specified--PIXC(1,1) and either a half life or a first order rate constant. For equilibrium and kinetics level 2, no constants need be specified--partition coefficients and rate constants are entered via parameters.

For kinetics level 3, some general chemical constants are usually available, as summarized in Table 4. MOLWT, SOLG, and VAPRG are sometimes used in volatilization computations, while LKOW can be used in sorption calculations.

If a chemical is ionic, then constants from Table 5 may be specified. For each ionic specie I, SPFLG(I) and PKA(I) must be specified. EPKA(I) may also be given. Ionic speciation is considered to be equilibrium level 5. The presence of ionic

species requires significantly more data specifications for the remaining processes.

Hydrophobic sorption at equilibrium levels may be simulated with constants from Table 6. If LKOC is unknown, then LKOW, AO, and A1 should be specified (if A0 and A1 are unknown, they default to log 0.6 and 1, respectively). NUX(1) and PIXC(I,1) should be left out. Solids-dependent partitioning constitutes equilibrium level 4. NUX(1) should be given a value of around 1. For equilibrium level 5, ionic sorption constants must also be specified. Their locations are given in Table 7.

For kinetics level 3, constants must be specified for each relevant process. Constants for volatilization, biodegradation, alkaline hydrolysis, neutral hydrolysis, acid hydrolysis, oxidation, and photolysis are given in Tables 8, 9, 11, 13, 15, 17, 19, and 20, respectively. Constants for a user-specified extra reaction are given in Table 22. If ionic speciation is being considered, then ionic rate constants must also be specified for each existing ionic specie. Locations of these constants are given in Tables 10, 12, 14, 16, 18, 21, and 23.

For kinetics level 4, reaction products are simulated. Four cases are illustrated in Figure 6.1 (in Part A of this manual). Yield coefficients for each relevant process must be specified. Yield coefficients for chemical 1, 2, and 3 reactions are listed in Tables 24, 25, and 26. The reactions themselves need not be second order to simulate reaction products.

TABLE 3 CONSTANTS FOR SIMPLE TOXI5 REACTIONS

Constant Number				
C_1	C_2	C_3	Variable	Definition
111	711	1311	PIXC(1,1)	Constant partition coefficient for sorption to solids (class 1), l_w/kgs
			K_i:	First order loss rate constants, day^{-1}
140	740	1340	KV	Volatilization
141	741	1341	KBW	Water column biodegradation
142	742	1342	KBS	Benthic biodegradation
181	781	1381	KHOH	Alkaline hydrolysis
182	782	1382	KHN	Neutral hydrolysis
183	783	1383	KHH	Acid hydrolysis
256	856	1456	KO	Oxidation
287	887	1487	KF	Photolysis
571	1171	1771	KE	Extra reaction
			TH_i	Half lives for reactions, day
143	743	1343	THBW	Water column biodegradation
144	744	1344	THBS	Benthic biodegradation
252	852	1452	THHOH	Alkaline hydrolysis
253	853	1453	THHN	Neutral hydrolysis
254	854	1454	THHH	Acid hydrolysis
257	857	1457	THO	Oxidation
289	889	1489	THF	Photolysis
572	1172	1772	THE	Extra reaction

TABLE 4 GENERAL CHEMICAL CONSTANTS

Constant Number				
C_1	C_2	C_3	Variable	Definition
9	609	1209	TDINT	Time interval at which rate constants are recomputed, days
81	681	1281	MOLWT	Molecular weight, g/mole
82	682	1282	SOLG	Solubility, mg/L
83	683	1283	VAPRG	Vapor pressure, torr
84	684	1284	LKOW	Log octanol-water partition coefficient, L_o/L_w

TABLE 5 IONIZATION CONSTANTS

Constant Number				
C_1	C_2	C_3	Variable	Definition
85	685	1285	SFLG(1)	flags indicating existence of ionic species +, ++, -, --; if SPFLG(I) = 1, ionic species I exists
86	686	1286	SFLG(2)	
87	687	1287	SFLG(3)	
88	688	1288	SFLG(4)	
91	691	1291	PKA(1)	For ionic species I, the constant in the integrated Van't Hoff equation describing temperature dependence of the equilibrium dependence of the equilibrium constant for dissociation: log K(I) = -PKA(I) + (EPKA(I)/2.303 R) * [$T*T_R/(T-T_R)$]
92	692	1292	PKA(2)	
93	693	1293	PKA(3)	
94	694	1294	PKA(4)	
95	695	1295	EPKA(1)	For ionic species I, the activation energy of the dissociation reaction, kcal/mole
96	696	1296	EPKA(2)	
97	697	1297	EPKA(3)	
98	698	1298	EPKA(4)	
99	699	1299	TREFI	Reference temperature at which dissociation reaction constants were measured, ˚C

TABLE 6 SORPTION CONSTANTS FOR TOTAL OR NEUTRAL CHEMICAL

Constant Number				
C_1	C_2	C_3	Variable	Definition
84	684	1284	LKOW	Log 10 of the octanol-water partition coefficient, log (L_w/L_o)
101	701	1301	LKOC	Log 10 of the organic carbon partition coefficient, log (L_w/kg_{oc})
102	702	1302	A0	Intercept in the K_{ow} - K_{oc} correlation: log K_{oc} = A0 · log K_{ow}; default = log 0.6
103	703	1303	A1	Slope in the K_{ow} - K_{oc} correlation; default = 1.0
106	706	1306	NUX(1)	Solids-dependent partitioning parameter ($_x$) of the chemical onto solids; default = 10^{12} makes K_p independent of solids concentration
111	711	1311	PIXC(1,1)	Solids-independent (limiting) partition coefficient K_{po} for sorption to solid 1, L_w/kg_s
116	716	1316	PIXC(2,1)	Solids-independent (limiting) partition coefficient K_{po} for sorption to solid 2, L_w/kg_s
121	721	1321	PIXC(3,1)	Solids-independent (limiting) partition coefficient K_{po} for sorption to solid 3, L_w/kg_s If = 0, K_{po} for neutral chemical will be calculated from LKOC and parameter FOC
--	--	--	PIDOC	Partition coefficient for DOC; for neutral chemical, KOC is used; L/kg

TABLE 7 LOCATION OF IONIC SORPTION CONSTANTS

Constant Number					
C_1	C_2	C_3	Variable	Ionic Specie	Sorptive Phase
106	706	1306	NUX(1)	0	S
107	707	1307	NUX(2)	+	S
108	708	1308	NUX(3)	++	S
109	709	1309	NUX(4)	-	S
110	710	1310	NUX(5)	--	S
111	711	1311	PIXC(1,1)	0	S1
112	712	1312	PIXC(1,2)	+	S1
113	713	1313	PIXC(1,3)	++	S1
114	714	1314	PIXC(1,4)	-	S1
115	715	1315	PIXC(1,5)	--	S1
116	716	1316	PIXC(2,1)	0	S2
117	717	1317	PIXC(2,2)	+	S2
118	718	1318	PIXC(2,3)	++	S2
119	719	1319	PIXC(2,4)	-	S2
120	720	1420	PIXC(2,5)	--	S2
121	721	1421	PIXC(3,1)	0	S3
122	722	1422	PIXC(3,2)	+	S3
123	723	1423	PIXC(3,3)	++	S3
124	724	1424	PIXC(3,4)	-	S3
125	725	1425	PIXC(3,5)	--	S3
126	726	1426	PIDOC(1)	+	B
127	727	1427	PIDOC(2)	++	B
128	728	1428	PIDOC(3)	-	B
129	729	1429	PIDOC(4)	--	B

TABLE 8 VOLATILIZATION CONSTANTS

Constant Number				
C_1	C_2	C_3	Variable	Definition
136	736	1336	XV	Volatilization option: 0 = no volatilization 1 = measured volatilization 2 = measured reaeration + O'Connor for gas transfer 3 = measured reaeration + MacKay for gas transfer 4 = calculated using O'Connor 5 = calculated using MacKay
137	737	1337	HENRY	Henry's constant, atm-m^3/mole
138	738	1338	KLT	Volatilization temperature correction factor, dimensionless
139	739	1339	KVOG	Measured ratio of volatilization to reaeration rates
2	2	2	WTYPE	Water body type (0 = flowing stream, river, or estuary; 1 = stagnant pond or lake)
5	5	5	AIRTMP	Multiplier for air temperature time function
8	608	1208	ATMOS	Atmospheric concentration of chemical, g/L

TABLE 9 SECOND ORDER BIODEGRADATION CONSTANTS FOR TOTAL FOR NEUTRAL CHEMICAL

Constant Number				
C_1	C_2	C_3	Variable	Definition
146	746	1346	KBIO20(1,1)	Second-order 20˚C biodegradation rate constant for aqueous, DOC-sorbed, and sediment-sorbed phases, mL/cells-day
151	751	1351	KBIO20(2,1)	
156	756	1356	KBIO20(3,1)	
161	761	1361	Q10DIS(1)	Temperature correction factor for biodegradation of aqueous, DOC-sorbed, and sediment-sorbed phases; multiplication factor for 10˚C temperature increase
166	766	1366	Q10DOC(1)	
171	771	1371	Q10PAR(1)	

TABLE 10 LOCATION OF IONIC BIODEGRADATION CONSTANTS

Constant Number					
C_1	C_2	C_3	Variable	Ionic Specie	Sorptive Phase
146	746	1346	KBIO20(1,1)	0	W
147	747	1347	KBIO20(1,2)	+	W
148	748	1348	KBIO20(1,3)	++	W
149	749	1349	KBIO20(1,4)	-	W
150	750	1350	KBIO20(1,5)	--	W
151	751	1351	KBIO20(2,1)	0	B
152	752	1352	KBIO20(2,2)	+	B
153	753	1353	KBIO20(2,3)	++	B
154	754	1354	KBIO20(2,4)	-	B
155	755	1355	KBIO20(2,5)	--	B
156	756	1356	KBIO20(3,1)	0	S
157	757	1357	KBIO20(3,2)	+	S
158	758	1358	KBIO20(3,3)	++	S
159	759	1359	KBIO20(3,4)	-	S
150	760	1460	KBIO20(3,5)	--	S
161	761	1461	Q10DIS(1)	0	W
162	762	1462	Q10DIS(2)	+	W
163	763	1463	Q10DIS(3)	++	W
164	764	1464	Q10DIS(4)	-	W
165	765	1465	Q10DIS(5)	--	W
166	766	1466	Q10DOC(1)	0	B
167	767	1467	Q10DOC(2)	+	B
168	768	1468	Q10DOC(3)	++	B
169	769	1469	Q10DOC(4)	-	B
170	770	1470	Q10DOC(5)	--	B
171	771	1471	Q10PAR(1)	0	S
172	772	1472	Q10PAR(2)	+	S

TABLE 10 LOCATION OF IONIC BIODEGRADATION CONSTANTS

Constant Number					
C_1	C_2	C_3	Variable	Ionic Specie	Sorptive Phase
173	773	1473	Q10PAR(3)	++	S
174	774	1474	Q10PAR(4)	-	S
175	775	1475	Q10PAR(5)	--	S

TABLE 11 SECOND ORDER ALKALINE HYDROLYSIS CONSTANTS FOR TOTAL OR NEUTRAL CHEMICAL

Constant Number				
C_1	C_2	C_3	Variable	Definition
184	784	1384	TREFH	Reference temperature at which hydrolysis rates were measured, ˚C
186	786	1386	KH2O(1,1,1)	Second order, 20˚C alkaline hydrolysis rate constants for aqueous, DOC-sorbed , and sediment-sorbed phases, L/mole-day
191	791	1391	KH2O(1,2,1)	
196	796	1396	KH2O(1,3,1)	
231	831	1431	EHOH(1)	Activation energy for alkaline hydrolysis, kcal/mole

TABLE 12 LOCATION OF IONIC ALKALINE HYDROLYSIS CONSTANTS

Constant Number					
C_1	C_2	C_3	Variable	Ionic Specie	Sorptive Phase
186	786	1386	KH2O(1,1,1)	0	W
187	787	1387	KH2O(1,1,2)	+	W
188	788	1388	KH2O(1,1,3)	++	W
189	789	1389	KH2O(1,1,4)	-	W
190	790	1390	KH2O(1,1,5)	--	W
191	791	1391	KH2O(1,2,1)	0	B
192	792	1392	KH2O(1,2,2)	+	B
193	793	1393	KH2O(1,2,3)	++	B
194	794	1394	KH2O(1,2,4)	-	B
195	795	1395	KH2O(1,2,5)	--	B
196	796	1396	KH2O(1,3,1)	0	S
197	797	1397	HK2O(1,3,2)	+	S
198	798	1398	KH2O(1,3,3)	++	S
199	799	1399	KH2O(1,3,4)	-	S
200	800	1400	KH2O(1,3,5)	--	S
231	831	1431	EHOH(1)	0	A
232	832	1432	EHOH(2)	+	A
233	833	1433	EHOH(3)	++	A
234	834	1434	EHOH(4)	-	A
235	835	1435	EHOH(5)	--	A

TABLE 13 SECOND ORDER NEURAL HYDROLYSIS CONSTANTS FOR TOTAL CHEMICAL

Constant Number				
C_1	C_2	C_3	Variable	Definition
184	784	1384	TREFH	Reference temperature at which hydrolysis rates were measured, ˚C
201	801	1401	KH2O(2,1,1)	20˚C neutral hydrolysis rate constant for aqueous, DOC-sorbed, and sediment-sorbed phases, day^{-1}
206	806	1406	KH2O(2,2,1)	
211	811	1411	KH2O(2,3,1)	
236	836	1436	EHN(1)	Activation energy for neutral hydrolysis, kcal/mole

TABLE 14 LOCATION OF IONIC NEUTRAL HYDROLYSIS CONSTANTS

Constant Number					
C_1	C_2	C_3	Variable	Ionic Specie	Sorptive Phase
201	801	1401	KH2O(1,1,2)	0	W
202	802	1402	KH2O(2,1,2)	+	W
203	803	1403	KH2O(3,1,2)	++	W
204	804	1404	KH2O(4,1,2)	-	W
205	805	1405	KH2O(5,1,2)	--	W
206	806	1406	KH2O(1,2,2)	0	B
207	807	1407	KH2O(2,2,2)	+	B
208	808	1408	KH2O(3,2,2)	++	B
209	809	1409	KH2O(4,2,2)	-	B
210	810	1010	KH2O(5,2,2)	--	B
211	811	1411	KH2O(1,3,2)	0	S
212	812	1412	KH2O(2,3,2)	+	S
213	813	1413	KH2O(3,3,2)	++	S
214	814	1414	KH2O(4,3,2)	-	S
215	815	1415	KH2O(5,3,2)	--	S
236	836	1436	EHN(1)	0	A
237	837	1437	EHN(2)	+	A
238	838	1438	EHN(3)	++	A
239	839	1439	EHN(4)	-	A
240	840	1440	EHN(5)	--	A

TABLE 15 SECOND ORDER ACID HYDROLYSIS CONSTANTS FOR TOTAL OR NEUTRAL CHEMICAL

Constant Number				
C_1	C_2	C_3	Variable	Definition
184	784	1384	TREFH	Reference temperature at which hydrolysis rates were measured, ˚C
216	816	1416	KH2O(3,1,1)	Second order, 20˚C acid hydrolysis rate constant for aqueous, DOC-sorbed and sediment-sorbed phases, L/mole-day
221	821	1421	KH2O(3,2,1)	
226	826	1426	KH2O(3,3,1)	
241	841	1441	EHH(1)	Activation energy for aced hydrolysis, kcal/mole

TABLE 16 LOCATION OF IONIC ACID HYDROLYSIS CONSTANTS

Constant Number					
C_1	C_2	C_3	Variable	Ionic Specie	Sorptive Phase
216	816	1416	KH2O(3,1,1)	0	W
217	817	1417	KH2O(3,1,2)	+	W
218	818	1418	KH2O(3,1,3)	++	W
219	819	1418	KH2O(3,1,4)	-	W
220	820	1420	KH2O(3,1,5)	--	W
221	821	1421	KH2O(3,2,1)	0	B
222	822	1422	KH2O(3,2,2)	+	B
223	823	1423	KH2O(3,2,3)	++	B
224	824	1424	KH2O(3,2,4)	-	B
225	825	1425	KH2O(3,2,5)	--	B
226	826	1426	KH2O(3,3,1)	0	S
227	827	1427	KH2O(3,3,2)	+	S
228	828	1428	KH2O(3,3,3)	++	S
229	829	1429	KH2O(3,3,4)	-	S
230	830	1430	KH2O(3,3,5)	--	S
241	841	1441	EHH(1)	0	A
242	842	1442	EHH(2)	+	A
243	843	1443	EHH(3)	++	A
244	844	1444	EHH(4)	-	A
245	845	1445	EHH(5)	--	A

TABLE 17 SECOND ORDER OXIDATION CONSTANTS FOR TOTAL OR NEUTRAL CHEMICAL

Constant Number				
C_1	C_2	C_3	Variable	Definition
258	858	1458	TREFO	Reference temperature at which oxidation rates were measured, ˚C
261	861	1461	KOX2O(1,1)	Second-order, 20˚C oxidation rate constant for aqueous, DOC-sorbed, and sediment-sorbed phases, L/mole-day
266	866	1466	KOX2O(2,1)	
271	871	1471	KOX2O(3,1)	
276	876	1476	EOX(1)	Activation energy for oxidation, kcal/mole

TABLE 18 LOCATION OF IONIC OXIDATION CONSTANTS

Constant Number					
C_1	C_2	C_3	Variable	Ionic Specie	Sorptive Phase
261	861	1461	KOX2O(1,1)	0	W
262	862	1462	KOX2O(2,1)	+	W
263	863	1463	KOX2O(3,1)	++	W
264	864	1464	KOX2O(4,1)	-	W
265	865	1465	KOX2O(5,1)	--	W
266	866	1466	KOX2O(1,2)	0	B
267	867	1467	KOX2O(2,2)	+	B
268	868	1468	KOX2O(2,2)	++	B
269	869	1469	KOX2O(4,2)	-	B
270	870	1470	KOX2O(5,2)	--	B
271	871	1471	KOX2O(1,3)	0	S
272	872	1472	KOX2O(2,3)	+	S
273	873	1473	KOX2O(3,3)	++	S
274	874	1474	KOX2O(4,3)	-	S
275	875	1475	KOX2O(5,3)	--	S
276	876	1476	EOX(1)	0	All
277	877	1477	EOX(2)	+	All
278	878	1478	EOX(3)	++	All
279	879	1479	EOX(4)	-	All
280	880	1480	EOX(5)	--	All

TABLE 19 TOXI5 PHOTOLYSIS CONSTANTS

Constant Number				
C_1	C_2	C_3	Variable	Definition
286	886	1486	XPHOTO	Photolysis option: 0 = no photolysis; 1 = computed from absorptivity; 2 = measured surface rate
288	888	1488	RFLATG	Latitude at which surface photolysis rate was measured, degree and tenths (option 2)
291	891	1491	KDPG(1)	Measured surface photolysis rate for neutral specie, day^{-1} (option 2)
296	896	1496	LAMAXG(1)	Wavelength of maximum light absorption for neutral specie, nm (option 2)
301-346	901-946	1501-1546	ABS(K,1,L)	Molar absorptivity of neutral specie of chemical K at wavelength number L, L/mole-cm-ln10 (option 1)
551	1151	1751	QUANTG(1,1)	Quantum yield of dissolved neutral chemical
556	1156	1756	QUANTG(1,2)	Quantum yield of dissolved neutral chemical
561	1161	1761	QUANTG(3,1)	Quantum yield of dissolved neutral chemical

L = Wavelength 1-46 (see Tables 7.12 and 7.13 in Part A of this document).

TABLE 20 GLOBAL CONSTANTS FOR TOXI5 PHOTOLYSIS OPTION 1

Constant Number				
C_1	C_2	C_3	Variable	Definition
1	601	1201	TO	Julian date at beginning of run
3	603	1203	ELEVG	Average ground surface elevation, m
4	604	1204	LATG	Latitude of water body, degrees
6	606	1206	XLITE	Water surface light intensity option; 0 = do not compute light; 1 = annual average; 2 = average for month indicated by TO; 3 = monthly step function
7	607	1207	DFACG	Ratio of optical path length to vertical depth; 1.17
11-23	611-623	1211-1223	CLOUDG(1)	Mean monthly cloudiness, in tenths of full sky coverage (0-10)
24-36	624-636	1224-1236	AIRTYG(1)	Mean monthly air mass type; 1 = rural, 2 = urban, 3 = maritime, 4 = tropospheric
37-49	637-649	1237-1249	RHUMG(1)	Mean monthly daylight relative humidity, percent
50-62	650-662	1250-1262	ATURBG(1)	Mean monthly atmospheric turbidity, in equivalent aerosol layer thickness km
63-75	663-675	1263-1275	OZONEG(1)	Mean monthly ozone content of atmosphere, in cm NTP (0.2 - 0.3)

TABLE 21 LOCATION OF IONIC PHOTOLYSIS CONSTANTS

Constant Number					
C_1	C_2	C_3	Variable	Ionic Specie	Sorptive Phase
291	891	1491	KDPG(1)	0	A
292	892	1492	KDPG(2)	+	A
293	893	1493	KDPG(3)	++	A
294	894	1494	KDPG(4)	-	A
295	895	1495	KDPG(5)	--	A
296	896	1496	LAMAXG(1)	0	A
297	897	1497	LAMAXG(2)	+	A
298	898	1498	LAMAXG(3)	++	A
299	899	1499	LAMAXG(4)	-	A
300	900	1500	LAMAXG(5)	--	A
301-346	901-946	1501-1546	ABS(K,1,L)	0	A
351-396	951-996	1551-1596	ABS(K,2,L)	+	A
401-446	1001-1046	1601-1646	ABS(K,3,L)	++	A
451-496	1051-1096	1561-1696	ABS(K,4,L)	-	A
501-546	1101-1146	1701-1746	ABS(K,5,L)	--	A
551	1151	1751	QUANTG(1,1)	0	W
552	1152	1752	QUANTG(1,2)	++	W
553	1153	1753	QUANTG(1,3)	+	W
554	1154	1754	QUANTG(1,4)	-	W
555	1155	1755	QUANTG(1,5)	--	W
556	1156	1756	QUANTG(2,1)	0	B
557	1157	1757	QUANTG(2,2)	+	B
558	11458	1758	QUANTG(2,3)	++	B
559	1159	1759	QUANTG(2,4)	-	B

TABLE 21 LOCATION OF IONIC PHOTOLYSIS CONSTANTS

Constant Number					
C_1	C_2	C_3	Variable	Ionic Specie	Sorptive Phase
560	1160	1760	QUANTG(2,5)	--	B
561	1161	1761	QUANTG(3,1)	0	S
562	1162	1762	QUANTG(3,2)	++	S
563	1163	1763	QUANTG(3,3)	+	S
564	1164	1764	QUANTG(3,4)	-	S
565	1165	1765	QUANTG(3,5)	--	S

TABLE 22 EXTRA SECOND ORDER REACTION CONSTANTS FOR TOTAL OR NEUTRAL CHEMICAL

Constant Number				
C_1	C_2	C_3	Variable	Definition
573	1173	1773	TREFE	Reference temperature at which extra reaction rates were measured, ˚C
576	1176	1776	KE2O(1,1)	Second-order, 20˚C extra reaction rate constant for aqueous, DOC-sorbed, and sediment-sorbed phases, 1/[E]-day
581	1181	1781	KE2O(2,1)	
586	1186	1786	KE2O(3,1)	
591	1191	1791	EEX(1)	Activation energy for extra reaction, kcal/mole

TABLE 23 LOCATION OF IONIC EXTRA REACTION CONSTANTS

Constant Number					
C_1	C_2	C_3	Variable	Ionic Specie	Sorptive Phase
576	1176	1776	KE2O(1,1)	0	W
577	1177	1777	KE2O(1,2)	+	W
578	1178	1778	KE2O(1,3)	++	W
579	1179	1779	KE2O(1,4)	-	W
580	1180	1780	KE2O(1,5)	--	W
581	1181	1781	KE2O(2,1)	0	B
582	1182	1782	KE2O(2,2)	+	B
583	1183	1783	KE2O(2,3)	++	B
584	1184	1784	KE2O(2,4)	-	B
585	1185	1785	KE2O(2,5)	--	B
586	1186	1786	KE2O(3,1)	0	S
587	1187	1787	KE20(3,2)	+	S
588	1188	1788	KE2O(3,3)	++	S
589	1189	1789	KE2O(3,4)	-	S
590	1190	1790	KE2O(3,5)	--	S
591	1191	1791	EEX(1)	0	All
592	1192	1792	EEX(2)	+	All
593	1193	1793	EEX(3)	++	All
594	1194	1794	EEX(4)	-	All
595	1195	1795	EEX(5)	--	All

TABLE 24 YIELD CONSTANTS FOR CHEMICAL 1 REACTIONS

Constant Number				
C_1	C_2	C_3	Variable	Definition
			Y( )12:	Yield coefficient for production of C_2 from C_1, mgC_2/mgC_1
176			YBW12	Water column biodegradation
178			YBS12	Benthic biodegradation
246			YHOH12	Alkaline hydrolysis
248			YHN12	Neutral hydrolysis
250			YHH12	Acid hydrolysis
281			YOX12	Oxidation
566			YF12	Photolysis
596			YE12	Extra reaction
			Y( )13:	Yield coefficient for production of C_3 from C_1, mgC_2/mgC_1
177			YBW13	Water column biodegradation
179			YBS13	Benthic biodegradation
247			YHOH13	Alkaline hydrolysis
249			YHN13	Neutral hydrolysis
251			YHH13	Acid hydrolysis
282			YOX13	Oxidation
567			YF13	Photolysis
597			YE13	Extra reaction

TABLE 25 YIELD CONSTANTS FOR CHEMICAL 2 REACTIONS

Constant Number				
C_1	C_2	C_3	Variable	Definition
			Y( )21:	Yield coefficient for production of C_1 from C_2, mgC_2/mgC_1
	776		YBW21	Water column biodegradation
	778		YBS21	Benthic biodegradation
	846		YHOH21	Alkaline hydrolysis
	848		YHN21	Neutral hydrolysis
	850		YHH21	Acid hydrolysis
	881		YOX21	Oxidation
	1166		YF21	Photolysis
	1196		YE21	Extra reaction
			Y( )23:	Yield coefficient for production of C_3 from C_2, mgC_3/mgC_2
	777		YBW23	Water column biodegradation
	779		YBS23	Benthic biodegradation
	847		YHOH23	Alkaline hydrolysis
	849		YHN23	Neutral hydrolysis
	851		YHH23	Acid hydrolysis
	882		YOX23	Oxidation
	1167		YF23	Photolysis
	1197		YE23	Extra reaction

TABLE 26 YIELD CONSTANTS FOR CHEMICAL 3 REACTIONS

Constant Number				
C_1	C_2	C_3	Variable	Definition
			Y( )31:	Yield coefficient for production of C_1 from C_3, mgC_1/mgC_2
		1376	YBW31	Water column biodegradation
		1378	YBS31	Benthic biodegradation
		1446	YHOH31	Alkaline hydrolysis
		1448	YHN31	Neutral hydrolysis
		1450	YHH31	Acid hydrolysis
		1481	YOX31	Oxidation
		1766	YF31	Photolysis
		1796	YE31	Extra reaction
			Y( )32:	Yield coefficient for production of C_2 from C_3, mgC_2/mgC_3
		1377	YBW32	Water column biodegradation
		1379	YBS32	Benthic biodegradation
		1447	YHOH32	Alkaline hydrolysis
		1449	YHN32	Neutral hydrolysis
		1451	YHH32	Acid hydrolysis
		1482	YOX32	Oxidation
		1767	YF32	Photolysis
		1797	YE32	Extra reaction

CHAPTER 10

DATA GROUP I: KINETIC TIME FUNCTIONS

The definition of the kinetic time functions will vary depending upon the structure and the kinetics of the systems comprising each model. The input format, however, is constant. Time functions are input as piecewise linear functions.

MDEP WASP provides additional time functions 24-35 (TEMP5-TEMP16) for parameter TMPFN and time function 36 (TFBOD) for parameter FBOD to allow CBOD fluxes.

10.1 RECORD FORMATS

Record 1--Number of Time Functions (I10, 70X)

NFUNC	=	number of time functions required by the model. If no time functions are to be input, set NFUNC equal to zero and go to Data Group J. (I10)
TITLE	=	name of data group. (70X)

Records 2-3 are input as a group NFUNC times:

Record 2--Time Function Descriptions (A5, 2I5)

ANAME(ISC)	=	an optional one to five alphanumeric character descriptive name for the time function I. (A5)
NOBRK(ISC)	=	number of breaks used to describe the time function I. (I5)
ISC	=	number identifying the time function; these numbers are set by the model developer. (I5)

Record 3--Time Functions (4(2F10.0))

VALT(K)	=	value of time function ISC at time T(K). (F10.0)
T(K)	=	time in days. If the length of the simulation exceeds T(NOBRK), the time function will repeat itself, starting at T(1), i.e., the approximation is assumed to

be periodic, with period equal to T(NOBRK). (F10.0)

Record 3 is repeated NOBRK(ISC)/4 times.

Record 1 in entered once in Data Group I. Records 2 and 3, as a set, are repeated NFUNC times. Within each NFUNC set, Record 2 is input once and Record 3 uses as many 80-space lines as needed to input NOBRK entries. Four entries (four VALK(K)-T(K) pairs) will fit on each 80-space line.

10.2 THE EUTROPHICATION MODEL

Listed below are the 36 time functions available for eutrophication in WASP 5.2-MDEP. Only TEMP(1) is required for Level 1 and 2 analyses. For Level 3 analyses, TFNH4, VELN(1), and WIND may be added (WIND is needed only for calculating reaeration in non-flowing water bodies such as lakes). For analyses at Level 4 and above, ITOT, F, KE, and TFPO4 should be used. For resolution of spatial variability in temperature, light extinction, and water velocity the four TEMP functions, the five KE functions, and the four VELN functions may be used.

Many of the time functions operate in conjuction with a parameter "pointer" in Data Group G. The parameter value specifies which of several time functions for temperature, light extinction, or water velocity are to be associated with each segment. Time functions 1-4 and 24-35 are the sixteen temperature functions available for parameter TMPFN. Time functions 8-12 are the five extinction coefficient functions for parameter KEFN. Functions 15-18 are the four water velocity options for VELFN. Time functions 24-35 (TEMP5-TEMP16) are the additional twelve (12) temperature functions available for parameter TMPFN and time function 36 (TFBOD) is added for parameter FBOD to allow CBOD fluxes in this upgraded WASP6.

ISC	ANAME	Defininion and Units
1	TEMP(1)	Time-variable temperature function 1. TEMP(K) can be either a normalized function or an actual temperature in ˚C, depending upon the definition of the parameter multiplier TMPSG(ISEG).
2	TEMP(2)	Time-variable temperature function 2, unitless or ˚C.

3	TEMP(3)	Time-variable temperature function 3, unitless or ˚C.
4	TEMP(4)	Time-variable temperature function 4, unitless or ˚C.
5	ITOT	Total daily solar radiation, langleys.
6	F	Fraction of day with sufficient light for growth, days.
7	WIND	Wind velocity, m/sec.
8	KE(1)	Time-variable extinction coefficient function 1. This can be either a normalized function or an actual extinction coefficient in m^{-1}, depending upon the definition of the parameter multiplier KESG(ISEG).
9	KE(2)	Time-variable extinction coefficient function 2, unitless or m^{-1}.
10	KE(3)	Time-variable extinction coefficient function 3, unitless or m^{-1}.
11	KE(4)	Time-variable extinction coefficient function 4, unitless or m^{-1}.
12	KE(5)	Time-variable extinction coefficient function 5, unitless or m^{-1}.
13	TFNH4	Normalized ammonium flux from bed, unitless.
14	TFPO4	Normalized phosphate flux from bed, unitless.
15	VELN(1)	Time variable velocity function 1, m/sec. This velocity is added to the net velocity VELOCG(ISEG) computed from the segment flow and the hydraulic parameters read in Data Group C.
16	VELN(2)	Time variable velocity function 2, m/sec.
17	VELN(3)	Time variable velocity function 3, m/sec.
18	VELN(4)	Time variable velocity function 4, m/sec.
19	ZOO	Herbivorous zooplankton population, mgC/L.
20	SALFN	Time variable salinity function, g/l. This function gets multiplied by the segment specific

		salinity multiplier entered in the parameter sector.
21	AIRTMP	Time variable ambient air temperature, ˚C. This provides air temperature data for the wind driven reaeration algorithms and is required.
22	XICEVR	This is the time variable ice cover function, %. This provides the percentage of water surface area available for reaeration. Note that 100% (entered as 1.0) indicates all surface area is available for reaeration.
23	REAR	Multiplier of parameter 14, REARSG, segment-specific oxygen reaeration rate constant
24	TEMP(5)	Time-variable temperature function 5. TEMP(K) can be either a normalized function or an actual temperature in ˚C, depending upon the definition of the parameter multiplier TMPSG(ISEG).
25	TEMP(6)	Time-variable temperature function 6, unitless or ˚C.
26	TEMP(7)	Time-variable temperature function 7, unitless or ˚C.
27	TEMP(8)	Time-variable temperature function 8, unitless or ˚C.
28	TEMP(9)	Time-variable temperature function 9, unitless or ˚C.
29	TEMP(10)	Time-variable temperature function 10, unitless or ˚C.
30	TEMP(11)	Time-variable temperature function 11, unitless or ˚C.
31	TEMP(12)	Time-variable temperature function 12, unitless or ˚C.
32	TEMP(13)	Time-variable temperature function 13, unitless or ˚C.
33	TEMP(14)	Time-variable temperature function 14, unitless or ˚C.
34	TEMP(15)	Time-variable temperature function 15, unitless or ˚C.

35	TEMP(16)	Time-variable temperature function 16, unitless or ˚C.
36	TFBOD	Normalized CBOD flux from bed, unitless.

10.3 THE TOXIC CHEMICAL MODEL

Listed below are the 17 time functions available in TOXI5. The parameters and time functions interact in such away to allow the user segment specific control of environmental data. For more details see the parameter input section.

Two of the time functions operate in conjuction with a parameter "pointer" in Data Group G. The parameter value specifies which of four time functions for temperature or water velocity are to be associated with each segment. Time functions 1-4 are the four temperature functions available for parameter TMPFN. Time functions 5-8 are the four water velocity options for VELFN.

ISC	ANAME	VALT(ISC)
1	TEMPN(1)	Time-variable temperature function 1. TEMPN(K) can be either a normalized function or an actual temperature in ˚C, depending upon the definition of the parameter multiplier TEMP(ISEG).
2	TEMPN(2)	Time variable temperature function 2, unitless or ˚C.
3	TEMPN(3)	Time variable temperature 3, unitless or ˚C.
4	TEMPN(4)	Time variable temperature 4, unitless or ˚C.
5	VELN(1)	Time variable velocity function 1, m/sec. This velocity is added to the net velocity VELOCG(ISEG) parameters read in Data Group C.
6	VELN(2)	Time variable velocity function 2, m/sec. This velocity is added to the net velocity VELOCG(ISEG) computed from the segment flow and the hydraulic parameters read in Data Group C.
7	VELN(3)	Time variable velocity function 3, m/sec. This velocity is added to the net velocity VELOCG(ISEG) computed from the segment flow and the hydraulic parameters read in Data Group C.

8	VELN(4)	Time variable velocity function 4, m/sec. This velocity is added to the net velocity VELOCG(ISEG) computed from the segment flow and the hydraulic parameters read in Data Group C.
9	WINDN	Time variable wind function, m/sec. This time function is multiplied by the segment specific wind multiplier WVEL entered in the parameter section.
10	PHNW	Time variable ph function. This time function is multiplied by the segment specific ph multiplier ph enter in the parameter section.
11	PHNS	Normalized benthic pH function, dimensionless. This is multiplied by the segment pH multiplier PH(ISEG) for benthic segments.
12	REARN	Time variable reaeration coefficient, per day. This variable is multiplied by the segment specific variable REAR. entered in the parameter section.
13	AIRTMPN	Air temperature, C. Used for calculating reaeration rate.
14	CHLN	Phytoplankton chlorophyll concentration, mg/l. This variable is multiplied by the segment specific variable CHPHL entered in the parameter section
15	PHTON	Normalized light intensity, dimensionless. This is used for photolysis option 2 to adjust the measured rate constant under controlled light intensity to a predicted rate constant under ambient light intensity.
16	BACNW	Time variable bacteria concentration in the water column, mg/l. This is multiplied by the segment specific multiplier BAC entered in the parameter section.
17	BACNS	Normalized benthic bacteria function, dimensionless. This is multiplied by the segment bacteria multiplier BAC(ISEG) for benthic segments.

For kinetics levels 1 and 2, no time functions need be specified. For kinetics level 3, time functions for each

relevant process may be specified. TEMPN can affect all reactions. Volatilization option 1 uses REARN. Volatilization options 4 and 5 use WINDN and AIRTMPN. Volatilization options 2 and 3 use either VELN or REARN. Photolysis option 1 uses CHLN; photolysis option 2 requires PHTON. Hydrolysis and ionization use PHNW and PHNS. Biodegradation uses BACNW and BACNS. Functions not specified default to 1.0.

CHAPTER 11

DATA GROUP J: INITIAL CONDITIONS

11.1 RECORD FORMATS

The initial conditions are the segment concentrations and densities for the state variables at time zero (the start of the simulation).

Records 1-2 are input as a group NOSYS times:

Record 1--System Information (A40, I5, F5.0, F10.0, 20X)

CHEML	=	chemical or system name (A40).
IFIELD	=	solids field (3, 4, or 5) that transports this system in its pure or sorbed form (I5).
DSED	=	density of system; 0.0 for chemical, 0.5-2.5 for solids, kg/L. (F5.0).
CMAX	=	maximum concentration allowed, mg/L. (F10.0)
TITLE	=	name of data group. (20X)

Record 2--Initial Conditions (3(A5, 2F10.0))

ANAME(K)	=	an optional one to five alphanumeric character descriptive name or number identifying segment K. (A5)
C(ISYS,K)	=	initial concentration in segment K of system ISYS in the appropriate units, mg/L. (F10.0)
DISSF	=	dissolved fraction of chemical in segment K. (F10.0)

Record 2 is repeated NOSEG/3 times.

Records 1 and 2 are a set and will be repeated NOSYS times. Within each NOSYS set, Record 2 will use as many 80-space lines as needed to input NOSEG entries. Three entries (ANAME-C-DISSF) will fit on one line. After NOSEG entries have been entered in a NOSYS set, begin the next NOSYS set on the following line. If ICFL = 2 in Data Group A, initial conditions are read from the

restart file (*.RST, where * is the input data set name), and Data Group J should not be included in the input data set.

11.2 THE EUTROPHICATION MODEL

Data Group J is input as a unit 9 times, once for each system. In record 1, solids transport fields must be specified for the particulate fraction of each system. In EUTRO5, solids field 3 is equated to particulate organic matter, solids field 4 is phytoplankton, and solids field 5 is inorganic sediment. The following specifications, then, are recommended for systems 1 through 8:

IFIELD(1) = 3 (solids field 1)

IFIELD(2) = 5 (solids field 3)

IFIELD(3) = 5 (solids field 3)

IFIELD(4) = 4 (solids field 2)

IFIELD(5) = 3 (solids field 1)

IFIELD(6) = 5 (solids field 3)

IFIELD(7) = 3 (solids field 1)

IFIELD(8) = 3 (solids field 1)

The density of each solid field must also be specified in record 1. This property is not used in EUTRO5. The user may enter 1.0 for the density of each system.

The dissolved fraction of each system in each segment must be specified in record 2. The user should take care to specify the dissolved fractions for dissolved oxygen (system 6) of 1.0 and the dissolved fractions for phytoplankton (system 4) of 0.0.

11.3 THE TOXIC CHEMICAL MODEL

Data Group J is input as a unit NOSYS times, once for each system. In record 1, solids transport fields must be specified for each solid (i.e.- variables 2, 3, and 4). While solids transport fields are also specified for each chemical (variables 1, 5, and 6), the values are nominal. TOXI5 will calculate the actual transport of the sorbed chemical fractions using internal partitioning relationships.

In Record 2, the dissolved fraction of each system in each segment must be specified. These values should be 1.0 for each solid variable (2, 3, and 4). Dissolved fraction values for each chemical are nominal. TOXI5 will calculate the actual dissolved fractions using internal partitioning relationships.

CHAPTER 12

WASP5 OUTPUT

12.1 GENERAL CONSIDERATIONS

WASP5 simulations produce several files that may be examined by the user. These files use the file name of the input data set with a unique extension. The most important of these are the simulation result files -- *.TDF for TOXI5 and *.EDF for EUTRO5 (i.e.- a TOXI5 input dataset named POND.INP produces an output file named POND.TDF). These formatted files contain all kinetic display variables for each segment at each print interval throughout the simulation. These display variables include state variable concentrations along with a selection of calculated variables and rates. Available display variables for EUTRO5 and TOXI5 are summarized in the eutrophication and toxics sections below.

The simulation results files can be processed with the post processing programs available with the WISP package or the W4DSPLY program which is provided with the mainframe version. The program will prompt the user for information.

Other files created by a WASP simulation include *.OUT, *.TRN, *.MSB, and *.RST (where * is the name of the input data set). The OUT file contains a record of the input data plus any simulation error messages that may have been generated. It may be examined from WISP by selecting the OUT file (alt-F, curser to OUT, return, escape) and using the BROWSE command from the menu.

The TRN file contains a set of transport-associated variables for each segment at each print interval throughout the simulation. These variables include the time step (day), calculated maximum time steps (day), segment volumes (m^3), segment flows (m^3/sec), flow changes (m^3/sec), time constants for segment flow (day^{-1}), segment exchange flows (m^3/sec), the time constant for segment exchanges (day^{-1}), the segment dispersion coefficient (m^3/sec), and the numerical dispersion coefficient (m^2/sec).

The MSB file contains a mass balance record for one designated system in the model network as a whole (in kg). For each print interval, this file records the accumulated mass in from advection, dispersion, and loading; the accumulated mass out through advection, dispersion, burial (or volatilization, and kinetic transformation; the total resident mass; and the residual (unaccounted for) mass.

The RST file contains a snapshot of volumes and concentrations of each system in each segment at the conclusion of the simulation. This file can be read by WASP5 to continue a series of simulations.

12.2 THE EUTROPHICATION MODEL

The standard WASP5 output files were summarized above. EUTRO5 stores in the EDF file 54 display variables. These variables are listed below. To examine these variables, the user may run WASP5 postprocessor.

EUTRO5 DISPLAY VARIABLES

Number	Variable	Definition
1	DEPTHG(I)	Segment Depth, m
2	STP	Water Temperature, ˚C
3	WIND	Wind Speed, m/sec
4	VEL	Water Velocity, m/sec
5	DO	Dissolved Oxygen, mg/L
6	DOMIN	DO Minimum, mg/L
7	DOMAX	DO Maximum, mg/L
8	CS	DO Saturation, mg/L
9	PERSAT	Percent DO Saturation, %
10	KA	Effective Reaeration Rate, day^{-1}
11	K2WSAVE	Wind Driven Reaeration, day^{-1}
12	K2HSAVE	Current Driven Reaeration, day^{-1}
13	SOD1D(I)	Sediment Oxygen Demand, g/m2/day
14	CBOD	CBOD, mg/L
15	BOD5	BOD5, mg/L
16	UBOD	Ultimate BOD, mg/L
17	TEMPBOD	BOD decay rate constant, day^{-1}
18	PHYT	Phytoplankton Carbon Biomass, mg/L
19	TCHLAX	Phytoplankton Chlorophyll **a**, g/L
20	GP1	Phytoplankton Growth Rate, day^{-1}

EUTRO5 DISPLAY VARIABLES

Number	Variable	Definition
21	DP1	Phytoplankton Death Rate, day^{-1}
22	SR19P	Phytoplankton DO Production, mg/L/day
23	SK19P	Phytoplankton DO Consumption, mg/L/day
24	CCHL1	Phyt. Carbon to Chl. **a** Ratio, mg/mg
25	RLGHTS(I,1)	Light Limit for Phyt. Growth
26	RNUTR	Nutrient Limit for Phyt. Growth
27	XEMP1	Nitrogen Limit for Phyt. Growth
28	XEMP2	Phosphorus Limit for Phyt. Growth
29	ITOTMP	Light at Segment Surface, langleys/day
30	IAV	Light at Top of Segment, langleys/day
31	IAVBOT	Light at Bottom of Segment, langleys/day
32	NH3	Ammonia Nitrogen, mg/L
33	NO3	Nitrate Nitrogen, mg/L
34	CN	Available Inorganic Nitrogen, mg/L
35	TON	Total Organic Nitrogen, mg/L
36	TIN	Total Inorganic Nitrogen, mg/L
37	TN	Total Nitrogen, mg/L
38	OPO4	Available Inorganic Phosphorus, mg/L
39	TIP	Total Inorganic Phosphorus, mg/L
40	TOP	Total Organic Phosphorus, mg/L
41	OP	Nonliving Organic Phosphorus, mg/L
42	SAL	Salinity, g/L
43	CMAC	Periphyton carbon biomass, mg/m^2 (normalized over total bottom area of segment)
44	GM1	Periphyton growth rate, day^{-1}
45	DM1	Periphyton death rate, day^{-1}
46	RS1	Periphyton respiration rate, day^{-1}

EUTRO5 DISPLAY VARIABLES

Number	Variable	Definition
47	SR19M	Periphyton DO Production, mg/L/day
48	SK19M	Periphyton DO Consumption, mg/L/day
49	RLGHTS2	Light Limit for Periphyton Growth
50	XEMP32	Density Limit for Periphyton Growth
51	XEMP22	Nitrogen Limit for Periphyton Growth
52	XEMP12	Phosphorus Limit for Periphyton Growth
53	CMMASS	Periphyton total mass (grams)
54	SA	Surface area (m^2)

12.3 THE TOXIC CHEMICAL MODEL

The standard WASP5 output files were summarized in Section 2.3. TOXI5 stores in the TDF file 18, 30, or 42 kinetic display variables, depending on whether 1, 2, or 3 chemicals were simulated. These variables are defined below. To examine these variables in tabular form, the user may run the WASP5 postprocessor as explained above.

TOXI5 DISPLAY VARIABLES

Constant Number				
C_1	C_2	C_3	Variable	Definition
1			TOTSOSL	Total solids concentration, mg/L
2			SOLID 1	Solids type 1 concentration, mg/L
3			SOLID 2	Solids type 2 concentration, mg/L
4			SOLID 3	Solids type 3 concentration, mg/L
5			STEMP	Segment temperature, ˚C
6			ITYPE	Segment type (1, 2, 3, or 4)
7	19	31	TOTCHEM	Total chemical concentration (1, 2, or 3), g/L

TOXI5 DISPLAY VARIABLES

Constant Number				
C_1	C_2	C_3	Variable	Definition
8	20	32	TOTDIS	Dissolved chemical concentration, g/L
9	21	33	TOTDOC	DOC-sorbed chemical concentration, g/L
10	22	34	TOTPAR	Total sorbed chemical concentration, g/L
11	23	35	TOTPAR1	Total sorbed chemical concentration, g/kg
12	24	36	TOTION	Total ionic chemical concentration, g/L
13	25	37	KBIO	Biodegradation rate constant, day^{-1}
14	26	38	KHYD	Total hydrolysis rate constant, day^{-1}
15	27	39	KFOT	Photolysis rate constant, day^{-1}
16	28	40	KVOL	Volatilization rate constant, day^{-1}
17	29	41	KOX	Oxidation rate constant, day^{-1}
18	30	42	KEXT	Extra rate constant, day^{-1}

12.4 EXCEL POST-PROCESSOR

As part of the development of the Maine DEP Version of WASP, a post-processor utility was developed. The post processor is programmed as a user-friendly 'data wizard' in Microsoft Excel. The post processor uses the plotting capabilities of Excel to plot program outputs selected by the user.

Use of the WASP Data Wizard is generally self explanatory. To start the program, the user should start the spreadsheet WASP Wizard.xls in Excel. A 'Run WASP data wizard' command button appears on the screen and the data wizard starts immediately. The user should follow instructions to select output from the water-quality output file (filetype .edf) or transport output file (filetype .trn), select the type of plot desired and the combination of output variables, simulation times, and segment locations desired, and make the plot. Upon the user selecting the 'Finish' command, the data wizard extracts the requested data from the output file, copies it into a new worksheet in Excel, and plots the data.

The user can create multiple plots in a single Excel file. Each time the user wants to add a new plot, he or she can return to the 'WASP Wizard' worksheet (tabbed at the bottom of the screen) and click on the 'Run WASP data wizard' command button. A new plot will be created in a new Excel worksheet.

The user may find it helpful to modify the resulting plots in Excel. The data and plots are entirely standard Excel content and can be manipulated accordingly. Sometimes in plotting multiple variables, highly disparate ranges lead to plots with a few variables plotted as essentially zero values while other variables dictate the axis limits. This problem can be corrected by selecting the mismatched data lines, right-clicking, selecting 'Format data series,' selecting 'Axis,' and finally selecting 'Secondary axis.' This sequence of commands will cause the creation of a new secondary axis on the right side of the graph that fits mismatched data series.